The term "protein tyrosine kinase," or PTK, refers to an enzyme that transfers the high energy phosphate of adenosine triphosphate to a tyrosine residue located on a protein target.

A protein tyrosine kinase catalytic domain of the invention can originate from receptor protein tyrosine kinases that bind fibroblast growth factor (FGF). These protein tyrosine kinases are known as "FGFR" herein, and can relate to one member of the FGFR family, such as FGFR1.

The term "catalytic domain" refers to the region of a protein that can exist as a separate entity from the protein. The catalytic domain of a protein tyrosine kinase is characterized as having considerable amino acid identity to the catalytic domain of other protein tyrosine kinases. Considerable amino acid identity preferably refers to at least 30% identity, more preferably at least 35% identity, and most preferably at least 40% identity. These degrees of amino acid identity refer to the identity between different protein tyrosine kinase families. Amino acid identity for members of a given protein tyrosine kinase family range from 55% to 90%. The catalytic domain may be functional as a separate entity. The catalytic domain of a protein tyrosine kinase is also characterized as a polypeptide that is soluble in solution.

The term "identity" identity as used herein refers to a property of sequences that measures their similarity or relationship. Identity is measured by dividing the number of identical residues in the two sequences by the total number of residues and multiplying the product by 100. Thus, two copies of exactly the same sequence have 100% identity, but sequences that are less highly conserved and have deletions, additions, or replacements have a lower degree of identity. Those skilled in the art will recognize that several computer programs are available for determining sequence identity.

The term "functional" refers to the ability of a catalytic domain to convert a substrate into a product by phosphorylating the substrate. The term "functional" also relates to the ability of a catalytic domain to bind natural binding partners. The catalytic region may comprise an N-terminal tail, a catalytic core, and a C-terminal tail. The catalytic core is a polypeptide that can be functional in terms of catalysis. N- and C-terminal tails are polypeptide regions that may not confer appreciable functionality in terms of catalysis, but may confer functionality in terms of modulator specificity.

A polypeptide can exist as a catalytic domain eventhough it is not functional. For example, a polypeptide corresponding to a catalytic domain may not be functional if it does not harbor phosphate moieties in key areas. Multiple examples of phosphorylation-state dependent function are well documented in the art. Therefore, a catalytic domain can also exist without being functional. A measure of a protein kinase catalytic domain is a polypeptide that is homologous to other protein kinase catalytic domains.

The term "polypeptide" refers to an amino acid chain representing a portion of, or the entire sequence of, amino acids comprising a protein.

A preferred embodiment of the invention includes a crystalline form of a PTK that is a receptor PTK. Receptors are proteins that straddle the inside and outside of the cell membrane. Receptor PTKs comprise an extracellular region, a transmembrane region, and an intracellular region comprising a catalytic domain.

Another preferred embodiment of the invention is the crystalline form of a receptor PTK selected from the group consisting of FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.

Yet another preferred embodiment of the invention is the crystalline form of a PTK that is a non-receptor PTK. Non-receptor PTKs are located inside the cell and do not harbor extracellular or membrane-spanning polypeptides attached to the polypeptide corresponding to the catalytic domain. Non-receptor PTKs may harbor fatty acids or lipids, which can impart a membrane associated character to a PTK. In preferred embodiments of the invention, crystalline forms of non-receptor PTKs are selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

In still another preferred embodiment, the invention features a crystalline form of a PTK that comprises a heavy metal atom. These types of crystals can be referred to as derivative crystals.

The term "derivative crystal" refers to a crystal where the polypeptide is in association with one or more heavy-metal atoms.

The term "association" refers to a condition of proximity between a chemical entity or compound, or portions or fragments thereof, and tyrosine kinase domain protein, or portions or fragments thereof. The association may be non-covalent, i.e., where the juxtaposition is energetically favored by, e.g., hydrogen-bonding, van der Waals, electrostatic or hydrophobic interactions, or it may be covalent.

The term "heavy metal atom" refers to an atom that is a transition element, a lanthanide metal, or an actinide metal. Lanthanide metals include elements with atomic numbers between 57 and 71, inclusive. Actinide metals include elements with atomic numbers between 89 and 103, inclusive.

In a preferred embodiment, the invention features a crystal of an FGF receptor tyrosine kinase domain protein. The FGF receptor tyrosine kinase domain protein can relate to FGFR1.

The term "FGFR1" refers to one member of multiple receptor PTKs that are homologous to one another and bind FGF. In this context, the term "homologous" refers to at least 70% amino acid identity between two members of the FGFR family.

The term "FGFR1" can also refer to a mutant of human FGFR1 which is characterized by the amino acid sequence of SEQ ID NO:2. As compared to human FGFR1, FGFR1 contains the following amino acid substitutions: Cys-488 → Ala, Cys-584 → Ser, Leu-457 → Val, and has an additional five amino acid residues at the N-terminus (Ser-Ala-Ala-Gly-Thr).

The term "human FGFR1" refers to the tyrosine kinase domain of human fibroblast growth factor receptor 1 ("FGFR1") having the amino acid sequence of SEQ ID

NO:1. Generally, human FGFR1 comprises a 310 amino acid residue fragment (residues 456 to 765) of human FGFR1.

The term "mutant" refers to a polypeptide which is obtained by replacing at least one amino acid residue in a native tyrosine kinase domain with a different amino acid residue. Mutation can be accomplished by adding and/or deleting amino acid residues within the native polypeptide or at the N- and/or C-terminus of a polypeptide corresponding to a native tyrosine kinase domain having substantially the same three-dimensional structure as the native tyrosine kinase domain from which it is derived. By having substantially the same three-dimensional structure is meant having a set of atomic structure coordinates that have a root mean square deviation (r.m.s.d.) of less than or equal to about 2 Å when superimposed with the atomic structure coordinates of the native tyrosine kinase domain from which the mutant is derived when at least about 50% to 100% of the Cα atoms of the native tyrosine kinase are included in the superposition. A mutant may have, but need not have, PTK activity.

In another preferred embodiment, the invention relates to a crystalline form defined by the structural coordinates set forth in Table 1.

The term "atomic structural coordinates" as used herein refers to a data set that defines the three dimensional structure of a molecule or molecules. Structural coordinates can be slightly modified and still render nearly identical three dimensional structures. A measure of a unique set of structural coordinates is the root-mean-square deviation of the resulting structure. Structural coordinates that render three dimensional structures that deviate from one another by a root-mean-square deviation of less than 1.5 Å may be viewed by a person of ordinary skill in the art as identical. Hence, the structural coordinates set forth in Table 1, Table 2, Table 3, and Table 4 are not limited to the values defined therein.

In other preferred embodiments, the invention features a crystalline form of the polypeptide in association with a compound. These types of crystalline forms can be referred to as co-crystals. The compound may be a cofactor, substrate, substrate analog, inhibitor, or allosteric effector.

The term "compound" refers to an organic molecule. The term "organic molecule" refers to a molecule which has at least one carbon atom in its structure. The compound can have a molecular weight of less than 6kDa. Both the geometry of the compound and the interactions formed between the compound and the polypeptide preferably govern high affinity binding between the two molecules. High affinity binding is preferably governed by a dissociation equilibrium constant on the order of $10^{-6}$ M or less. The compound is preferably a modulator that alters the function of a PTK.

The term "function," in reference to the effect of a modulator on PTK function, refers to the ability of a modulator to enhance or inhibit the catalytic activity of a PTK.

The term "catalytic activity", in the context of the invention, defines the ability of a PTK to phosphorylate a substrate polypeptide. Catalytic activity can be measured, for example, by determining the amount of a substrate converted to a product as a function of time. The conversion of the substrate to a product occurs at the active-site of the PTK.

The term "active-site" refers to a cavity located in the PTK in which one or more substrate molecules may bind. Addition of a modulator to cells expressing a PTK may enhance (activate) or lower (inhibit) the catalytic activity of the PTK.

A small number of inhibitors of PTK catalytic activity are known in the art. Small molecule inhibitors may modulate PTK function by blocking the binding of substrates. Indolinone compounds, for example, may bind to the active-site of PTK catalytic domains and inhibit them effectively, as measured by inhibition constants on the order of $10^{-6}$ M or less.

Activators of PTK intracellular regions can enhance PTK function by interacting with both the PTK catalytic domain and the substrate. Activators may also promote dimerization of PTKs and thus activate them by bringing them into close proximity with one another. In addition, activators may operate by promoting a conformational change in the intracellular region of the PTK such that the catalytic region modifies substrates at a faster rate in the presence of the activator.

The term "function" can also refer to the ability of a modulator to enhance or inhibit the association between a PTK and a natural binding partner.

The term "natural binding partner" refers to a polypeptide that normally binds to a PTK in a cell. These natural binding partners can play a role in propagating a signal in a PTK signal transduction process. The natural binding partner can bind to a PTK with high affinity. High affinity represents an equilibrium binding constant on the order of $10^{-6}$ M or less. However, a natural binding partner can also transiently interact with a PTK and chemically modify it. PTK natural binding partners are chosen from a group consisting of, but not limited to, *src* homology 2 (SH2) or 3 (SH3) domains, other phosphoryl tyrosine binding (PTB) domains, nucleotide exchange factors, and other protein kinases or protein phosphatases.

The term "interactions" refers to hydrophobic, aromatic, and ionic forces and hydrogen bonds formed between atoms in the modulator and the enzyme active-site.

The term "cofactor" refers to a compound that may, in addition to the substrate, bind to a protein and undergo a chemical reaction. Multiple co-factors are nucleotides or nucleotide derivatives, such as phosphate and nicotinamide derivatives of adenosine.

The term "substrate" refers to a compound that reacts with an enzyme. Enzymes can catalyze a specific reaction on a specific substrate. For example, PTKs can phosphorylate specific protein and peptide substrates on tyrosine moieties. In addition, nucleotides can act as substrates for protein kinases.

The term "substrate analog" refers to a compound that is structurally similar, but not identical, to a substrate. The substrate analog may be a nucleotide analog. Examples of nucleotide analogs are described below.

The term "inhibitor" refers to a compound that decreases the cellular function of a protein kinase. The protein kinase function is preferably the interaction with a natural binding partner and more preferably catalytic activity.

The term "allosteric effector" refers to a compound that causes allosteric interactions in a protein. The term "allosteric interactions" refers to interactions between separate sites on a protein. The sites can be different from the active site. The allosteric effector can enhance or inhibit catalytic activity by binding to a site that may be different than the active site.

The term "co-crystal" refers to a crystal where the polypeptide is in association with one or more compounds.

In preferred embodiments, a co-crystal of the invention can be in association with a heavy metal atom. Examples of heavy metal atoms are described above.

In other preferred embodiments, the invention features a co-crystal comprising the crystalline form of the polypeptide in association with a compound, where the compound is a non-hydrolyzable analog of ATP. These analogs can be referred to as nucleotide analogs.

The term "ATP" refers to the chemical compound adenosine triphosphate.

The term "non-hydrolyzable" refers to a compound having a covalent bond that does not readily react with water. Examples of non-hydrolyzable analogs of ATP are AMP-PNP and AMP-PCP, whose structures are well known to those skilled in the art.

The term "AMP-PNP" refers to adenylyl

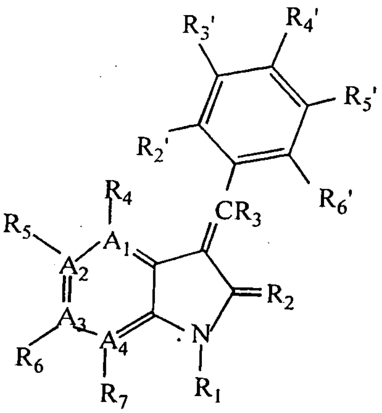
imidodiphosphate, a non-hydrolyzable analog of ATP.

The term "AMP-PCP" refers to adenylyl diphosphonate, a non-hydrolyzable analogue of ATP.

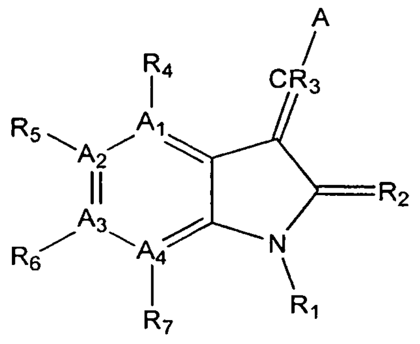
In another preferred embodiment, the invention relates to a crystalline form defined by the structural coordinates set forth in Table 2.

In preferred embodiments, the invention relates to crystalline forms, where the compound in association with the polypeptide is an indolinone.

Certain indolinones are specific modulators of PTK function. A preferred embodiment of the invention is the crystalline form of a PTK complexed with an indolinone of formula I or II:



(I)



(II)

or a pharmaceutically acceptable salt, isomer, metabolite, ester, amide, or prodrug thereof, where:

(a) $A_1$, $A_2$, $A_3$, and $A_4$ are independently carbon or nitrogen;

(b) $R_1$ is hydrogen or alkyl;

(c) $R_2$ is oxygen in the case of an oxindolinone or sulfur in the case of a thiolindolinone;

(d) $R_3$ is hydrogen;

(e) $R_4$, $R_5$, $R_6$, and $R_7$ are optionally present, and are either (i) independently selected from the group consisting of alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, $SO_2NRR'$, $SO_3R$, SR, $NO_2$, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, $(CH_2)_nCO_2R$, and CONRR' or (ii) any two adjacent $R_4$, $R_5$, $R_6$, and $R_7$ taken together form a fused ring with the aryl portion of the indole-based portion of the indolinone;

(f) $R_2'$, $R_3'$, $R_4'$, $R_5'$, and $R_6'$ are each independently selected from the group consisting of hydrogen, alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, $SO_2NRR'$, $SO_3R$, SR, $NO_2$, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, $(CH_2)_nCO_2R$, and CONRR';

(g) n is 0, 1, 2, or 3;

(h) R is hydrogen, alkyl or aryl;

(i) R' is hydrogen, alkyl or aryl; and

(j) A is a five membered heteroaryl ring selected from the group consisting of thiophene, pyrrole, pyrazole, imidazole, 1,2,3-triazole, 1,2,4-triazole, oxazole, isoxazole, thiazole, isothiazole, furan, 1,2,3-oxadiazole, 1,2,4-oxadiazole, 1,2,5-oxadiazole, 1,3,4-oxadiazole, 1,2,3,4-oxatriazole, 1,2,3,5-oxatriazole, 1,2,3-thiadiazole, 1,2,4-thiadiazole, 1,2,5-thiadiazole, 1,3,4-thiadiazole, 1,2,3,4-thiatriazole, 1,2,3,5-thiatriazole, and tetrazole, optionally substituted at one or more positions with alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, $SO_2NRR'$, $SO_3R$, SR, $NO_2$, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, $(CH_2)_nCO_2R$ or CONRR'.

The term "pharmaceutically acceptable salt" refers to those salts which retain the biological activity and properties of the free bases. Pharmaceutically acceptable salts can be obtained by reaction with inorganic acids such as hydrochloric acid, hydrobromic acid, sulfuric acid, nitric acid, phosphoric acid, methanesulfonic acid, ethanesulfonic acid, p-toluenesulfonic acid, salicylic acid and the like.

The term "prodrug" refers to an agent that is converted into the parent drug *in vivo*. Prodrugs may be easier to administer than the parent drug in some situations. For example, the prodrug may be bioavailable by oral administration but the parent is not, or the prodrug may improve solubility to allow for intravenous administration.

"Alkyl" refers to a straight-chain, branched or cyclic saturated aliphatic hydrocarbon. Preferably, the alkyl group has 1 to 12 carbons. More preferably, it is a lower alkyl of from 1 to 7 carbons, more preferably 1 to 4 carbons. Typical alkyl groups include methyl, ethyl, propyl, isopropyl, butyl, isobutyl, tertiary butyl, pentyl, hexyl and the like. The alkyl group may be optionally substituted with one or more substituents are selected from the group consisting of hydroxyl, cyano, alkoxy, =O, =S, $NO_2$, halogen, $N(CH_3)_2$ amino, and SH.

"Alkenyl" refers to a straight-chain, branched or cyclic unsaturated hydrocarbon group containing at least one carbon-carbon double bond. Preferably, the alkenyl group has 2 to 12 carbons. More preferably it is a lower alkenyl of from 2 to 7 carbons, more preferably 2 to 4 carbons. The alkenyl group may be optionally substituted with one or more substituents selected from the group consisting of hydroxyl, cyano, alkoxy, =O, =S, $NO_2$, halogen, $N(CH_3)_2$ amino, and SH.

"Alkynyl" refers to a straight-chain, branched or cyclic unsaturated hydrocarbon containing at least one carbon-carbon triple bond. Preferably, the alkynyl group has 2 to 12 carbons. More preferably it is a lower alkynyl of from 2 to 7 carbons, more preferably 2 to 4 carbons. The alkynyl group may be optionally substituted with one or more substituents selected from the group consisting of hydroxyl, cyano, alkoxy, =O, =S, $NO_2$, halogen, $N(CH_3)_2$ amino, and SH.

"Alkoxy" refers to an "O-alkyl" group.

"Aryl" refers to an aromatic group which has at least one ring having a conjugated pi-electron system and includes carbocyclic aryl, heterocyclic aryl and biaryl groups. The aryl group may be optionally substituted with one or more substituents selected from the group consisting of halogen, trihalomethyl, hydroxyl, SH, OH, $NO_2$, amine, thioether, cyano, alkoxy, alkyl, and amino.

"Alkaryl" refers to an alkyl that is covalently joined to an aryl group. Preferably, the alkyl is a lower alkyl.

"Carbocyclic aryl" refers to an aryl group wherein the ring atoms are carbon.

"Heterocyclic aryl" refers to an aryl group having from 1 to 3 heteroatoms as ring atoms, the remainder of the ring atoms being carbon. Heteroatoms include oxygen, sulfur, and nitrogen. Thus, heterocyclic aryl groups include furanyl, thienyl, pyridyl, pyrrolyl, N-lower alkyl pyrrolo, pyrimidyl, pyrazinyl, imidazolyl and the like.

"Amide" refers to -C(O)-NH-R, where R is alkyl, aryl, alkylaryl or hydrogen.

"Thioamide" refers to -C(S)-NH-R, where R is alkyl, aryl, alkylaryl or hydrogen.

"Amine" refers to a -N(R')R'' group, where R' and R'' are independently selected from the group consisting of alkyl, aryl, and alkylaryl.

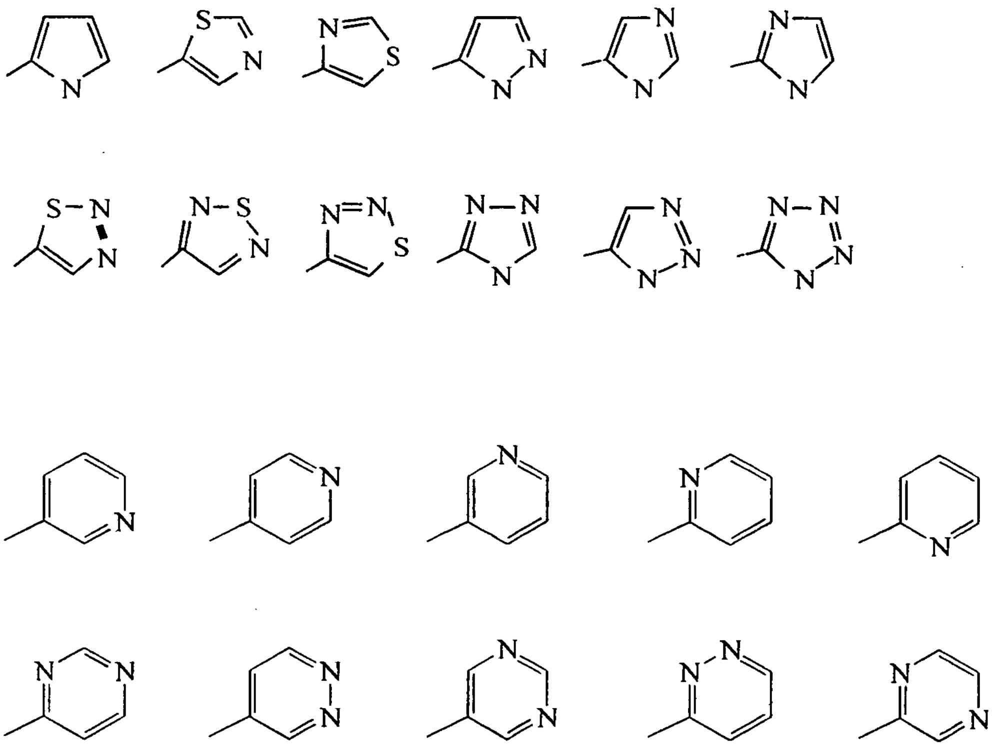
"Thioether" refers to -S-R, where R is alkyl, aryl, or alkylaryl.

"Sulfonyl" refers to $-S(O)_2-R$, where R is aryl, C(CN)=C-aryl, $CH_2CN$, alkyaryl, sulfonamide, NH-alkyl, NH-alkylaryl, or NH-aryl.

The term "acyl" denotes groups -C(O)R, where R is alkyl as defined above, such as formyl, acetyl, propionyl, or butyryl.

It is understood by those skilled in the art that when $A_1$, $A_2$, $A_3$, and $A_4$ are nitrogen or sulfur that the corresponding $R_4$, $R_5$, $R_6$, and $R_7$, as well as the corresponding bond, do not exist.

Examples of indoles having such fused rings (as described in (e) (ii) above include the following:



The six membered rings shown above exemplify possible A rings in compound II.

Other preferred embodiments of the invention are crystalline forms comprising 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone as well as 3-[4-(4-formylpiperazine-1-yl-)benzylidenyl]-2-indolinone. The polypeptide of these crystalline forms can be FGFR, and specifically, FGFR1.

In preferred embodiments, the crystalline forms of the invention can be defined by the structural coordinates set forth in Table 3 or Table 4.

The use of X-ray crystallography can elucidate the three dimensional structure of crystalline forms of the invention. The first characterization of crystalline forms by X-ray crystallography can determine the unit cell shape and its orientation in the crystal.

In other preferred embodiments, the invention features a crystal of an FGF receptor tyrosine kinase domain protein, where the crystal is characterized by having monoclinic unit cells. The crystal may also be characterized by having space group symmetry C2.

The term "unit cell" refers to the smallest and simplest volume element (i.e., parallelpiped-shaped block) of a crystal that is completely representative of the unit of pattern of the crystal. The dimensions of the unit cell are defined by six numbers: dimensions a, b and c and angles $\alpha$, $\beta$ and $\gamma$. A crystal can be viewed as an efficiently packed array of multiple unit cells. Detailed descriptions of crystallographic terms are described in, which is hereby incorporated herein by reference in its entirety, including any drawings, figures, and tables.

The term "monoclinic unit cell" refers to a unit cell where $a \neq b \neq c$; $\alpha = \gamma = 90°$; and $\beta > 90°$.

The term "space group" refers to the symmetry of a unit cell. In a space group designation (e.g., C2) the capital letter indicates the lattice type and the other symbols represent symmetry operations that can be carried out on the unit cell without changing its appearance.

The term "lattice" in reference to crystal structures refers to the array of points defined by the vertices of packed unit cells.

The term "symmetry operations" refers to geometrically defined ways of exchanging equivalent parts of a unit cell, or exchanging equivalent molecules between two different unit cells. Examples of symmetry operations are screw axes, centers of inversion, and mirror planes.

In a preferred embodiment, the invention features a crystalline form, where the monoclinic unit cells have dimensions of about a=208.3 Å, b=57.8 Å, c=65.5 Å and $\beta$=107.2°.

In a preferred embodiment, the invention features a FGFR1 crystal, where the monoclinic unit cells have dimensions of about a=211.6 Å, b=51.3 Å, c=66.1 Å and $\beta$=107.7°.

In another aspect the invention features a polypeptide corresponding to the catalytic domain of a protein tyrosine kinase, containing at least about 20 amino acid residues upstream of the first glycine in the conserved glycine-rich region of the catalytic domain, and at least about 17 amino acid residues downstream of the conserved arginine located at the C-terminal boundary of the catalytic domain.

The polypeptides of the invention can be isolated, enriched or purified. In addition, the crystalline forms of the invention can be formed from polypeptides that are isolated, enriched, or purified.

By "isolated" in reference to a polypeptide is meant a polymer of 6, 12, 18 or more amino acids conjugated to each other, including polypeptides that are isolated from a natural source or that are synthesized. The isolated polypeptides of the present invention are unique in the sense that they are not found in a pure or separated state in nature. Use of the term "isolated" indicates that a naturally occurring sequence has been removed from its normal cellular environment. Thus, the sequence may be in a cell-free solution or placed in a different cellular environment. The term does not imply that the sequence is the only amino acid chain present, but that it is essentially free (about 90 - 95% pure at least) of material naturally associated with it.

By the use of the term "enriched" in reference to a polypeptide it is meant that the specific amino acid sequence constitutes a significantly higher fraction (2 - 5 fold) of the total of amino acids present in the cells or solution of interest than in normal or diseased cells or in the cells from which the sequence was taken. This could be caused by a person by preferential reduction in the amount of other amino acids present, or by a preferential increase in the amount of the specific amino acid sequence of interest, or by a combination of the two. However, it should be noted that “enriched” does not imply that there are no other amino acid sequences present, just that the relative amount of the sequence of interest has been significantly increased. The term significant here is used to indicate that the level of increase is useful to the person making such an increase, and generally means an increase relative to other amino acids of about at least 2 fold, more preferably at least 5 to 10 fold or even more. The term also does not imply that there are no amino acids from other sources. The other source amino acids may, for example, comprise amino acids encoded by a yeast or bacterial genome, or a cloning vector such as pUC19. The term is meant to cover only those situations in which a person has intervened to elevate the proportion of the desired nucleic acid.

It is also advantageous for some purposes that an amino acid sequence be in purified form. The term "purified" in reference to a polypeptide does not require absolute purity (such as a homogeneous preparation); instead, it represents an indication that the sequence is relatively purer than in the natural environment (compared to the natural level this level should be at least 2-5 fold greater, *e.g.*, in terms of mg/ml). Purification of at least one order of magnitude, preferably two or three orders, and more preferably four or five orders of magnitude is expressly contemplated. The substance is preferably free of contamination at a functionally significant level, for example 90%, 95%, or 99% pure.

In a preferred embodiment, the invention features a polypeptide corresponding to the catalytic domain of a receptor PTK. The receptor PTK may have a three-dimensional structure substantially similar to that of the insulin receptor, even though the amino acid content may be different.

In a preferred embodiment, the invention features a polypeptide corresponding to the catalytic domain of a non-receptor PTK, where the non-insulin receptor tyrosine kinase is a cytoplasmic tyrosine kinase.

In a preferred embodiment, the invention features a polypeptide corresponding to the catalytic domain of a receptor PTK, selected from the group consisting of FGF-R, PDGF-R, KDR, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, or MUSK.

In a preferred embodiment, the invention features a polypeptide corresponding to the catalytic domain of a non-receptor PTK, selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, or ACK.

In a preferred embodiment, the invention features a polypeptide corresponding to the catalytic domain of a PTK, having the amino acid sequence shown in Table 1 or Table 2.

In another aspect, the invention features a method for creating crystalline forms described herein. The method may utilize the polypeptides described herein to form a crystal. The method comprises the steps of:

(a) mixing a volume of polypeptide solution with a reservoir solution; and

(b) incubating the mixture obtained in step (a) over the reservoir solution in a closed container, under conditions suitable for crystallization.

These processes are described in detail in the section entitled "Detailed Description of the Invention."

In another aspect, the invention features a method of obtaining FGF receptor tyrosine kinase domain polypeptide in crystalline form, comprising the steps of: (a) mixing a volume of polypeptide solution with an equal volume of reservoir solution, where the polypeptide solution comprises 1 mg/mL to 60 mg/mL FGF-type tyrosine kinase domain protein, 10 mM to 200 mM buffering agent, 0 mM to 20 mM dithiothreitol and has a pH of about 5.5 to about 7.5, and where the reservoir solution comprises 10% to 30% (w/v) polyethylene glycol, 0.1 M to 0.5 M ammonium sulfate, 0% to 20% (w/v) ethylene glycol or glycerol, 10 mM to 200 mM buffering agent and has a pH of about 5.5 to about 7.5; and (b) incubating the mixture obtained in step (a) over said reservoir solution in a closed container at a temperature between 0° and 25°C until crystals form.

In a preferred embodiment, the invention features a method of obtaining FGF receptor tyrosine kinase domain polypeptide in crystalline form, where the polypeptide solution comprises about 10 mg/mL FGF receptor tyrosine kinase domain, about 10 mM sodium chloride, about 2 mM dithiothreitol, about 10 mM Tris-HCl and has a pH of about 8; the reservoir buffer comprises about 16% (w/v) polyethylene glycol (MW 10000), about 0.3 M ammonium sulfate, about 5% ethylene glycol or glycerol, about 100 mM bis-Tris and has a pH of about 6.5; and the temperature is about 4°C.

In another preferred embodiment, the invention features a method of obtaining FGF receptor tyrosine kinase domain polypeptide in crystalline form, where the polypeptide solution includes a compound such as a cofactor, substrate, substrate analog, inhibitor or allosteric effector.

In still another preferred embodiment, the invention features a method of obtaining FGF receptor tyrosine kinase domain polypeptide in crystalline form, where the compound is a nucleotide analog, such as a non-hydrolyzable analog of ATP, or an indolinone. Indolinone compounds have the general structural formula as described herein.

In another aspect, the invention features a cDNA encoding an FGF receptor tyrosine kinase domain protein, where a coding strand of the cDNA has the nucleotide sequence of SEQ ID NO:5.

Another aspect of the invention relates to a method of determining three dimensional structures of PTKs with unknown structure by utilizing the structural coordinates of Table 1, Table 2, Table 3, and Table 4. These methods can relate to homology modeling, molecular replacement, and nuclear magnetic resonance methods.

In a preferred embodiment, the invention relates to a method of determining three dimensional structures of PTKs with unknown structures by utilizing the coordinates of Table 1, Table 2, Table 3, or Table 4 in conjunction with the amino acid sequences of PTKs. This method of homology modeling comprises the steps of: (a) aligning the computer representation of an amino acid sequence of a PTK with unknown structure with that of a PTK with known structure, where alignment is achieved by matching homologous regions of the amino acid sequences;

(b) transferring the computer representation of an amino acid structure in the PTK sequence of known structure to a computer representation of a structure of the corresponding amino acid in the PTK sequence with unknown structure; and (c) determining low energy conformations of the resulting PTK structure.

The term "amino acid sequence" describes the order of amino acids in the amino acid chain comprising a polypeptide corresponding to the catalytic domain of a PTK.

The term "aligning" describes matching the beginning and the end of two or more amino acid sequences. Homologous amino acid sequences are placed on top of one another during the alignment process.

The term "homologous" describes amino acids in two sequences that are identical or have similar side-chain chemical groups (*e.g.*, aliphatic, aromatic, polar, negatively charged, or positively charged).

The term "corresponding" refers to an amino acid that is aligned with another in the sequence alignment mentioned above.

The term "determining the low energy conformation" describes a process of changing the conformation of the PTK structure such that the structure is of low free energy. The PTK structure may or may not have molecules, such as modulators bound to it.

The term "low free energy" describes a state where the molecules are in a stable state as measured by the process. A stable state is achieved when favorable interactions are formed within the complex.

The term "favorable interactions" refers to hydrophobic, aromatic, and ionic forces, and hydrogen bonds.

Another preferred embodiment of the invention relates to a method of determining three dimensional structures of PTKs with unknown structure. This method is accomplished by applying the structural coordinates of Table 1, Table 2, Table 3, or Table 4 to an incomplete X-ray crystallographic data set for a PTK. The method comprises the steps of: (a) aligning the positions of atoms in the unit cell by matching electron diffraction data from two crystals, where one data set is complete and the other is incomplete; and (b) determining a low energy conformation of the resulting PTK structure.

The term "incomplete data set" relates to a X-ray crystallographic data set that does not have enough information to give rise to a three dimensional structure.

In another preferred embodiment, the invention relates to a method of determining three dimensional structures of PTKs with unknown structure by applying the structural coordinates of Table 1, Table 2, Table 3, or Table 4 to nuclear magnetic resonance (NMR) data of a PTK. This method comprises the steps of: (a) determining the secondary structure of a PTK structure using NMR data; and (b) simplifying the assignment of through-space interactions of amino acids. The PTK structure may not be complexed with compounds or modulators.

The term "secondary structure" describes the arrangement of amino acids in a three dimensional structure, such as in α-helix or β-sheet elements.

The term "through-space interactions" defines the orientation of the secondary structural elements in the three dimensional structure and the distances between amino acids from different portions of the amino acid sequence.

The term "assignment" defines a method of analyzing NMR data and identifying which amino acids give rise to signals in the NMR spectrum.

In another aspect, the invention features a method of identifying potential modulators of PTK function. These modulators are identified by docking a computer representation of a structure of a compound with a computer representation of a cavity formed by the active-site of a PTK. The computer representation of the PTK active-site structure can be defined by structural coordinates.

The term "chemical group" refers to moieties that can form hydrogen bonds, hydrophobic, aromatic, or ionic interactions.

The term "docking" refers to a process of placing a compound in close proximity with a PTK. The term can also refer to a process of finding low energy conformations of the compound/PTK complex.

A preferred embodiment of the invention is a method of identifying potential modulators of PTK function. The method involves utilizing the structural coordinates or a PTK three dimensional structure. The structural coordinates set forth in Table 1, Table 2, Table 3, and Table 4 can be utilized. The method comprises the steps of: (a) removing a computer representation of a PTK structure and docking a computer representation of a compound from a computer data base with a computer representation of the active-site of the PTK; (b) determining a conformation of the complex with a favorable geometric fit and favorable complementary interactions; and (c) identifying compounds that best fit the PTK active-site as potential modulators of PTK function. The initial PTK structure may or may not have compounds bound to it.

The term "favorable geometric fit" refers to a conformation of the compound-PTK complex where the surface area of the compound is in close proximity with the surface area of the active-site without forming unfavorable interactions. Unfavorable interactions can be steric hindrances between atoms in the compound and atoms in the PTK active-site.

The term "favorable complementary interactions" relates to hydrophobic, aromatic, ionic, and hydrogen bond donating, and hydrogen bond accepting forces formed between the compound and the PTK active-site.

The term "potential" qualifies the term "modulator of PTK function" because the potential modulator or PTK function has not yet been tested for activity *in vitro* or *in vivo*.

The term "best fit" describes compounds that complexed the most surface area in the complex and/or form the most favorable complementary interactions with the PTK in the screen in a given experiment.

Another preferred embodiment of the invention is a method of identifying potential modulators of PTK function. The method involves utilizing a three dimensional structure of a PTK, with or without compounds bound to it. The method comprises the steps of: (a) modifying a computer representation of a PTK having one or more compounds bound to it, where the computer representations of the compound or compounds and PTK are defined by structural coordinates; (b) determining a conformation of the complex with a favorable geometric fit and favorable complementary interactions; and (c) identifying the compounds that best fit the PTK active-site as potential modulators of PTK function.

The term "modifying" relates to deleting a chemical group or groups or adding a chemical group or groups. Computer representations of the chemical groups can be selected from a computer data base.

Yet another preferred embodiment of the invention is a method of identifying potential modulators of PTK function by operating modulator construction or modulator searching computer programs on the compounds complexed with the PTK. The method comprises the steps of: (a) removing a computer representation of one or more compounds complexed with a PTK; and (b) searching a data base for compounds similar to the removed compounds using a compound searching computer program, or replacing portions of the compounds complexed with the PTK with similar chemical structures from a data base using a compound construction computer program, where the representations of the compounds are defined by structural coordinates.

The term "operating" as used herein refers to utilizing the three-dimensional conformation of molecules defined by the processes described herein in various computer programs.

The term "similar compound" refers to a compound in a computer data base that has a similar geometric structure as compounds that can bind to a PTK. The similar compound can also have similar chemical groups as the compounds that are either bound to the PTK or once bound to the PTK. The similar chemical groups can form complementary interactions with the PTK.

The term "compound searching computer program" describes a computer program that searches computer representations of compounds from a computer data base that have similar three dimensional structures and similar chemical groups as a compound of interest. The compound of interest is preferably an indolinone compound.

The term "similar chemical structures" refers to chemical groups that share similar geometry as portions of the compounds in complex with the PTK or compounds removed from the PTK structure. Similar chemical structures can also refer to chemical groups that may form similar complementary interactions as portions of the compounds in complex with the PTK or compounds removed from the PTK structure.

The term "replacing structures" refers to removing a portion of the compounds in complex with the PTK or compounds removed from the PTK structure and connecting the broken bonds to a similar chemical structure.

The term "compound construction computer program" describes a computer program that replaces computer representations of chemical groups in a compound with groups from a computer data base. The compound is preferably an indolinone compound.

The term "similar three dimensional structure" describes two molecules with nearly identical shape and volume.

In another preferred embodiment of the invention, the PTK structures used in the modulator design or identification method of the invention are defined by the structural coordinates of Table 1, Table 2, Table 3, or Table 4.

The methods for using the crystalline forms and three dimensional structures of the invention can relate to a broad range of protein kinases. Thus, in preferred embodiments, the invention relates to a receptor PTK. The receptor PTK can be selected form the group consisting of FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK. The PTK may also exist as a non-receptor PTK. The non-receptor PTK can be selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

In another aspect, the invention features a potential modulator of PTK function identified by methods disclosed in the invention.

A preferred embodiment of the invention is that the potential modulator of PTK function is an oxindolinone or a thiolindolinone of formula I or II disclosed above.

Another aspect of the invention is a method for synthesizing a potential modulator of PTK function or its pharmaceutically acceptable salts, isomers, metabolites, esters, amides, or prodrugs by a standard synthetic method known in the art. Synthetic procedures are discussed below.

In another aspect, the invention features a method of identifying a potential modulator of PTK function as a modulator of PTK function. The method comprises the steps of: (a) administering a potential modulator of PTK function to cells; (b) comparing the level of PTK phosphorylation between cells not administered the potential modulator and cells administered the potential modulator; and (c) identifying the potential modulator as a modulator of PTK function based on the difference in the level of PTK phosphorylation.

The term "cells" refers to any type of cells either primary or cultured. Primary cells can be extracted directly from an organism while cultured cells rapidly divide and can be cultured in many successive rounds. Cells can be grown in a variety of containers including, but not limited to flasks, dishes, and well plates.

The term "administer" refers to a method of delivering a compound to cells. The compound can be prepared using a carrier such as dimethyl sulfoxide (DMSO) in an aqueous solution. The aqueous solution comprising the compound, also termed an "aqueous preparation", can be simply mixed into the medium bathing the layer of cells or microinjected into the cells themselves. The compounds may be administered to the cells using a suitable buffered solution.

The term "suitable buffered solution" refers to an aqueous preparation of the compound that comprises a salt that can control the pH of the solution at low concentrations. Because the salt exists at low concentrations, the salt preferably does not alter the function of the cells.

The term "PTK phosphorylation" refers to the presence of phosphate on the PTK. Phosphates on PTKs can be identified by antibodies that bind them specifically with high affinity.

In another aspect, the invention features a method of identifying a potential modulator of PTK function as a modulator of PTK function. The method comprises the steps of: (a) administering a potential modulator of PTK function to cells; (b) comparing the level of cell growth between cells not administered the potential modulator and cells administered the potential modulator; and (c) identifying the potential modulator as a modulator of PTK function based on the difference in cell growth.

The term "cell growth" refers to the rate at which a group of cells divides. Cell division rates can be readily measured by methods utilized by those skilled in the art.

Another aspect of the invention features a method of diagnosing a disease by identifying cells harboring a PTK with inappropriate activity. The method comprises the steps of: (a) administering a modulator of PTK function to cells; (b) comparing the rate of cell growth between cells not administered the modulator and cells administered the modulator; and (c) diagnosing a disease by characterizing cells harboring a PTK with inappropriate activity from the effect of the modulator on the difference in the rate of cell growth. The modulator can be identified by the methods of the invention.

The term "inappropriate activity" refers to a PTK that regulates a step in a signal transduction process at a higher or lower rate than normal cells. Aberrations in the rate of signal transduction can be caused by alterations in the stimulation of a receptor PTK by a growth factor, alterations in the activity of PTK-specific phosphatase, over-expression of a PTK in a cell, or mutations in the catalytic region of the PTK itself.

The term "signal transduction process" describes the steps in a cascade of events where an extracellular signal is transmitted into an intracellular signal.

The term "PTK-specific phosphatase" describes an enzyme that dephosphorylates a particular PTK and thereby regulates that PTK's activity.

Another aspect of the invention is a method of treating a disease associated with a PTK with inappropriate activity in a cellular organism, where the method comprises the steps of: (a) administering the modulator of PTK function to the organism, where the modulator is in an acceptable pharmaceutical preparation; and (b) activating or inhibiting the PTK function to treat the disease.

The term "organism" relates to any living being comprised of at least one cell. An organism can be as simple as one eukaryotic cell or as complex as a mammal.

The term "administering", in reference to an organism, refers to a method of introducing the compound to the organism. The compound can be administered when the cells or tissues of the organism exist within the organism or outside of the organism. Cells existing outside the organism can be maintained or grown in cell culture dishes. For cells harbored within the organism, many techniques exist in the art to administer compounds, including (but not limited to) oral, parenteral, dermal, and injection applications. For cells outside of the patient, multiple techniques exist in the art to administer the compounds, including (but not limited to) cell microinjection techniques, transformation techniques, and carrier techniques.

The term "pharmaceutically acceptable composition" refers to a preparation comprising the modulator of PTK activity. The composition is acceptable if it does not appreciably cause irritations to the organism administered the compound.

Preferred embodiments of the of the invention are that the PTK is a receptor PTK selected from the group consisting of FGF-R, PDGF-R, FLK-1, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK. Other preferred embodiments of the invention are that the PTK is a non-receptor PTK selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

The summary of the invention described above is non-limiting and other features and advantages of the invention will be apparent from the following detailed description, and from the claims.

## BRIEF DESCRIPTION OF THE FIGURES

FIG. 1 provides a ribbon diagram of the structure of FGFR1 showing the side chains of tyrosines Tyr-653 and Tyr-654 and the α helical (αC, αD, αE, αEF, αF-αI), β strand (β1-β5, β7, β8), nucleotide-binding loop, catalytic loop, activation loop and kinase insert regions of the molecule. The termini are denoted by N and C. The loop between β2 and β3 is disordered, indicated by a break in the chain in this region.

FIG. 2 provides a stereo view of a $C_\alpha$ trace of FGFR1 shown in the same orientation as FIG. 1, with every tenth amino acid residue marked with a filled circle and every twentieth amino acid residue labeled with a residue number.

FIG. 3 provides a structure-based sequence alignment of human fibroblast growth factor receptor 1 (FGFR1), human fibroblast growth factor receptor 2 (FGFR2), human fibroblast growth factor receptor 3 (FGFR3), human fibroblast growth factor receptor 4 (FGFR4), a *D. malanogaster* homolog (DFGFR1), a *C. elegans* homolog (EGL-15) and insulin receptor tyrosine kinase (IRK).

FIGS. 4A and 4B provide ribbon diagrams of the N-terminal lobes (4A) and C-terminal lobes (4B) of FGFR1 and IRK in which the $C_\alpha$ atoms of the β sheets (4A) or α-helices (4B) of the two proteins have been superimposed.

FIG. 5 illustrates the side-chain positions of the tyrosine autophosphorylation sites of FGFR1 on the backbone representation of FGFR1.

FIGS. 6A and 6B are amino acid sequence alignments of the catalytic domains of PTKs, including receptor and non-receptor type PTKs. FIG. 6A depicts one representative member from each of the eighteen subfamilies of receptor tyrosine kinases. FIG. 6B depicts one representative member from each of the subfamilies of cytoplasmic tyrosine kinases. In FIGS. 6A and 6B highly conserved residues are boxed. The position of the glycine-rich domain, kinase insert, catalytic loop, and activation loop are indicated. The numbering is for human FGF-receptor.

## BRIEF DESCRIPTION OF THE CRYSTALLOGRAPHIC ATOMIC STRUCTURAL COORDINATES

The crystallographic structural coordinates are located at the end of the section entitled "Examples" and before the claims. Three sets of coordinates can be found in the Protein Data Bank under accession names 1FGK, 1AGW, and 1FGI. The 1FGK coordinates correspond to those listed in Table 1, the 1AGW coordinates correspond to those listed in Table 4, and the 1FGI coodinates correspond to those listed in Table 3. The 1AGW and 1FGI coordinate sets will be publically available in March 1998.

Table 1 provides the atomic structure coordinates of native FGFR1 crystals of the invention as determined by X-ray crystallography; and

Table 2 provides the atomic structure coordinates of FGFR1:AMP-PCP co-crystals of the invention as determined by X-ray crystallography.

Table 3 lists crystallographic coordinates defining the three dimensional structure of FGF-R1 complexed with 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone. The columns (from left to right) are descriptions of the atoms by number and type, amino acid and number containing the atom, the x coordinate, y coordinate, z coordinate, bond connectivity, and temperature factor. All of these parameters are well defined in the art.

Table 4 is a file of crystallographic coordinates defining the three dimensional structure of FGF-R1 complexed with 3-[4-(4-formylpiperazine-1-yl) benzylidenyl]-2-indolinone. The columns are as described in Table 3.

## DETAILED DESCRIPTION OF THE INVENTION

The present invention is directed to the design and identification of modulators of protein tyrosine kinase function that are PTK subfamily specific, non-hydrolyzable under acidic conditions, and highly bioavailable. The three dimensional structures of a PTK optionally complexed with compounds can facilitate design and identification of modulators of PTK function.

Protein tyrosine kinases (PTKs) comprise a large and diverse class of enzymes. Schlessinger and Ullrich, 1992, *Neuron 9*: 383-391. The PTK family is subdivided into members that are receptors and those that are non-receptors. The PTK receptor family contains multiple subfamilies, one of which is the fibroblast growth factor receptor (FGF-R) PTK which is a molecule implicated in regulating angiogenesis a well as cellular proliferation and differentiation. Givol and Yayon, 1992, *FASEB J. 6 (15)*: 3362-3369.

FGF-R1 can mediates cellular functions by its role in one or more cellular signal transduction processes. Cellular signal transduction processes comprise multiple steps that convert an extracellular signal into an intracellular signal.

Receptor PTK mediated signal transduction is initiated by binding a specific extracellular ligand, followed by receptor dimerization, and subsequent autophosphorylation of the receptor PTK. The phosphate groups are binding sites for intracellular signal transduction molecules which leads to the formation of protein complexes at the cell membrane. These complexes facilitate an appropriate cellular effect (*e.g.*, cell division, metabolic effects to the extracellular microenvironment) in response to the ligand that began the cascade of events.

Receptor PTKs function as binding sites for several intracellular proteins. Intracellular PTK binding proteins are divided into two principal groups: (1) those which harbor a catalytic domain; and (2) those which lack such a domain but serve as adapters and associate with catalytically active molecules. Songyang *et al.*, 1993, *Cell 72*:767-778. SH2 (*src* homology) domains are common adaptors found in proteins which directly bind to the receptor PTK. SH2 domains are harbored by PTK binding proteins of both groups mentioned above. Fantl *et al.*, 1992, *Cell 69*:413-423; Songyang *et al.*, 1994, *Mol. Cell. Biol. 14*:2777-2785); Songyang *et al.*, 1993, *Cell 72*:767-778; and Koch *et al.*, 1991, *Science 252*:668-678.

The specificity of the interactions between receptor PTKs and the SH2 domains of their binding proteins is determined by the amino acid residues immediately surrounding the phosphorylated tyrosine residue. Differences in the binding affinities of SH2 domains is correlated with the observed differences in substrate phosphorylation profiles of downstream molecules in the signal transduction process. Songyang *et al.*, 1993, *Cell* 72:767-778. These observations suggest that the function of each receptor PTK is determined not only by its pattern of expression and ligand availability but also by the array of downstream signal transduction pathways that are activated by a particular receptor. Thus, PTKs provide a controlling regulatory role in signal transduction processes as a consequence of autophosphorylation.

PTK-mediated signal transduction regulates cell proliferative, differentiation, and metabolic responses in cells. Therefore, inappropriate PTK activity can result in a wide array of disorders and diseases. These disorders, which are described below, may be treated by the modulators of PTK function designed or identified by the methods disclosed herein.

The present invention also relates to crystalline polypeptides corresponding to the catalytic domain of receptor tyrosine kinases. Such tyrosine kinases include receptors of a class that are not covalently cross-linked but are understood to undergo ligand-induced dimerization, as well as cytoplasmic tyrosine kinases. Preferably, the crystalline catalytic domains are of sufficient quality to allow for the determination of a three-dimensional X-ray diffraction structure to a resolution of about 1.5 Å to about 2.5 Å. The invention also relates to methods for preparing and crystallizing the polypeptides. The polypeptides themselves, as well as information derived from their crystal structures can be used to analyze and modify tyrosine kinase activity as well as to identify compounds that interact with the catalytic domain.

The polypeptides of the invention are designed on the basis of the structure of a region in the cytoplasmic domain of the receptor tyrosine kinase that contains the catalytic domain. By way of illustration, FIG. 6A shows the amino acid sequence alignment of the catalytic domains of eighteen human receptor tyrosine kinases; one representative member from each of the eighteen subfamilies is shown. FIG. 6B shows the alignment for cytoplasmic kinases. The applicants have discovered and determined the boundaries of the domain required for crystallization of the resulting polypeptide. Surprisingly, these boundaries differ from that required for catalytic activity. For example, referring to FIG. 6A, the domain required for catalytic activity is generally believed to span about 7 amino acid residues upstream of the first glycine (FIG. 6A residue number 485) of the N-terminal glycine-rich region through about 10 residues beyond the C-terminal conserved arginine (FIG. 6A, residue number 744). However, the additional sequence upstream of the N-terminal glycine-rich region and downstream of the C-terminal conserved arginine can be required for crystallization. In particular, at least about 20 amino acid residues (+/- 5 amino acid residues) upstream of the first glycine (<u>i.e.</u>, FIG. 6A, residue number 485) in the conserved glycine-rich region of the catalytic domain, and at least about 17 amino acid residues (+/- 5 amino acid residues) downstream of the conserved arginine (i.e., FIG. 6A, residue number 744) located at the C-terminal boundary of the catalytic domain can be required to engineer a polypeptide suitable for crystallization.

In those situations where the resulting polypeptide contains cysteine residues that interfere with crystallization (e.g., cysteine residue numbers 488 and 584 in the FGF-R1 sequence shown in FIG. 6A), such cysteine residues can be substituted with an appropriate amino acid that does not readily form covalent bonds with other amino acid residues under crystallization conditions; e.g., by substituting the cysteine with Ala, Ser or Gly. Any cysteine located in a non-helical or non-β-stranded segment, based on secondary structure assignments, are good candidates for replacement. For example, cysteines located in regions corresponding to the glycine-rich-loop, the kinase insert, the juxtamembrane region or the activation loop are prime candidates for replacement. However, substitutions of cysteine residues that are conserved among the kinases (e.g., FIG. 6A at positions 725 and 736) are preferably avoided.

## I. PTK Associated Diseases

Blood vessel proliferative disorders refer to angiogenic and vasculogenic disorders generally resulting in abnormal proliferation of blood vessels. The formation and spreading of blood vessels play important roles in a variety of physiological processes such as embryonic development, corpus luteum formation, wound healing and organ regeneration. They also play a pivotal role in cancer development. Other examples of blood vessel proliferation disorders include arthritis, where new capillary blood vessels invade the joint and destroy cartilage, and ocular diseases, like diabetic retinopathy, where new capillaries in the retina invade the vitreous, bleed and cause blindness. Conversely, disorders related to the shrinkage, contraction or closing of blood vessels are implicated in such diseases as restenosis.

Fibrotic disorders refer to the abnormal formation of extracellular matrix. Examples of fibrotic disorders include hepatic cirrhosis and mesangial cell proliferative disorders. Hepatic cirrhosis is characterized by the increase in extracellular matrix constituents resulting in the formation of a hepatic scar. Hepatic cirrhosis can cause diseases such as cirrhosis of the liver. An increased extracellular matrix resulting in a hepatic scar can also be caused by viral infection such as hepatitis.

Mesangial cell proliferative disorders refer to disorders brought about by abnormal proliferation of mesangial cells. Mesangial proliferative disorders include various human renal diseases, such as glomerulonephritis, diabetic nephropathy, malignant nephrosclerosis, thrombotic microangiopathy syndromes, transplant rejection, and glomerulopathies. The PDGF-R has been implicated in the maintenance of mesangial cell proliferation. Floege *et al.*, 1993, *Kidney International* 43:47S-54S.

PTKs are directly associated with the cell proliferative disorders described above. For example, some members of the receptor PTK family have been associated with the development of cancer. Some of these receptors, like EGFR (Tuzi *et al.*, 1991, *Br. J. Cancer 63*:227-233; Torp *et al.*, 1992, *APMIS 100*:713-719) HER2/neu (Slamon *et al.*, 1989, *Science 244*:707-712) and PDGF-R (Kumabe *et al.*, 1992, *Oncogene* 7:627-633) are over-expressed in many tumors and/or persistently activated by autocrine loops. In fact, PTK over-expression (Akbasak and Suner-Akbasak *et al.*, 1992, *J. Neurol. Sci. 111*:119-133; Dickson *et al.*, 1992, *Cancer Treatment Res. 61*:249-273; Korc *et al.*, 1992, *J. Clin. Invest. 90*:1352-1360) and autocrine loop stimulation (Lee and Donoghue, 1992, *J. Cell. Biol. 118*:1057-1070; Korc *et al.*, *supra*; Akbasak and Suner-Akbasak *et al.*, *supra*) account for the most common and severe cancers. For example, EGFR is associated with squamous cell carcinoma, astrocytoma, glioblastoma, head and neck cancer, lung cancer and bladder cancer. HER2 is associated with breast, ovarian, gastric, lung, pancreas and bladder cancer. PDGF-R is associated with glioblastoma, lung, ovarian, melanoma and prostate cancer. The receptor PTK c-met is generally associated with hepatocarcinogenesis and thus hepatocellular carcinoma. Additionally, c-met is linked to malignant tumor formation. More specifically, c-met has been associated with, among other cancers, colorectal, thyroid, pancreatic and gastric carcinoma, leukemia and lymphoma. Additionally, over-expression of the c-met gene has been detected in patients with Hodgkins disease, Burkitts disease, and the lymphoma cell line.

The IGF-I receptor PTK, in addition to being implicated in nutritional support and in type-II diabetes, is also associated with several types of cancers. For example, IGF-I has been implicated as an autocrine growth stimulator for several tumor types, *e.g.* human breast cancer carcinoma cells (Arteaga *et al.*, 1989, *J. Clin. Invest. 84*:1418-1423) and small lung tumor cells (Macauley *et al.*, 1990, *Cancer Res. 50*:2511-2517). In addition, IGF-I, integrally involved in the normal growth and differentiation of the nervous system, appears to be an autocrine stimulator of human gliomas. Sandberg-Nordqvist *et al.*, 1993, *Cancer Res. 53*:2475-2478. The importance of the IGF-IR and its modulators in cell proliferation is further supported by the fact that many cell types in culture (fibroblasts, epithelial cells, smooth muscle cells, T-lymphocytes, myeloid cells, chondrocytes, osteoblasts, the stem cells of the bone marrow) are stimulated to grow by IGF-I. Goldring and Goldring, 1991, *Eukaryotic Gene Expression 1*:301-326. In a series of recent publications suggest that IGF-IR plays a central role in the mechanisms of transformation and, as such, could be a preferred target for therapeutic interventions for a broad spectrum of human malignancies. Baserga, 1995, *Cancer Res. 55*:249-252; Baserga, 1994, *Cell 79*:927-930; Coppola *et al.*, 1994, *Mol. Cell. Biol. 14*:4588-4595.

The association between abnormalities in receptor PTKs and disease are not restricted to cancer, however. For example, receptor PTKs are associated with metabolic diseases like psoriasis, diabetes mellitus, wound healing, inflammation, and neurodegenerative diseases. EGF-R is indicated in corneal and dermal wound healing.

Defects in Insulin-R and IGF-IR are indicated in type-II diabetes mellitus. A more complete correlation between specific receptor PTKs and their therapeutic indications is set forth in Plowman *et al.*, 1994, *DN&P* 7:334-339.

Non-receptor PTKs, including src, abl, fps, yes, fyn, lyn, lck, blk, hck, fgr, yrk (reviewed by Bolen *et al.*, 1992, *FASEB J.* 6:3403-3409), are involved in the proliferative and metabolic signal transduction pathways also associated with receptor PTKs. Therefore, the present invention is also directed towards designing modulators against this class of PTKs. For example, mutated src (v-src) is an oncoprotein ($pp60^{v\text{-}src}$) in chicken. Moreover, its cellular homolog, the proto-oncogene $pp60^{c\text{-}src}$ transmits oncogenic signals of many receptors. For example, over-expression of EGF-R or HER2/neu in tumors leads to the constitutive activation of $pp60^{c\text{-}src}$, which is characteristic of the malignant cell but absent in the normal cell. On the other hand, mice deficient for the expression of c-src exhibit an osteopetrotic phenotype, indicating a key participation of c-src in osteoclast function and a possible involvement in related disorders. Similarly, Zap 70 is implicated in T-cell signaling. Both receptor PTKs and non-receptor PTKs are connected to hyperimmune disorders.

The instant invention is directed in part towards designing modulators of PTK function that could indirectly kill tumors by cutting off their source of sustenance. Normal vasculogenesis and angiogenesis play important roles in a variety of physiological processes such as embryonic development, wound healing, organ regeneration and female reproductive processes such as follicle development in the corpus luteum during ovulation and placental growth after pregnancy. Folkman and Shing, 1992, *J. Biological Chem.* *267*:10931-34. However, many diseases are driven by persistent unregulated or inappropriate angiogenesis. For example, in arthritis, new capillary blood vessels invade the joint and destroy the cartilage. In diabetes, new capillaries in the retina invade the vitreous, bleed and cause blindness. Folkman, 1987, in: *Congress of Thrombosis and Haemostasis* (Verstraete, *et. al*, eds.), Leuven University Press, Leuven, pp.583-596. Ocular neovascularization is the most common cause of blindness and dominates approximately twenty (20) eye diseases.

Moreover, vasculogenesis and/or angiogenesis can be associated with the growth of malignant solid tumors and metastasis. A tumor must continuously stimulate the growth of new capillary blood vessels for the tumor itself to grow. Furthermore, the new blood vessels embedded in a tumor provide a gateway for tumor cells to enter the circulation and to metastasize to distant sites in the body. Folkman, 1990, *J. Natl. Cancer Inst.* *82*:4-6; Klagsbrunn and Soker, 1993, *Current Biology* *3*:699-702; Folkman, 1991, *J. Natl., Cancer Inst.* *82*:4-6; Weidner *et al.*, 1991, *New Engl. J. Med.* *324*:1-5.

Several polypeptides with *in vitro* endothelial cell growth promoting activity have been identified. Examples include acidic and basic fibroblastic growth factor (αFGF, βFGF), vascular endothelial growth factor (VEGF) and placental growth factor. Unlike αFGF and βFGF, VEGF has recently been reported to be an endothelial cell specific mitogen. Ferrara and Henzel, 1989, *Biochem. Biophys. Res. Comm. 161*:851-858; Vaisman *et al.*, 1990, *J. Biol. Chem. 265*:19461-19566.

Thus, identifying the specific receptors that bind FGF or VEGF is important for understanding endothelial cell proliferation regulation. Two structurally related receptor PTKs that bind VEGF with high affinity are identified: the flt-1 receptor (Shibuya *et al.*, 1990, *Oncogene 5*:519-524; De Vries *et al.*, 1992, *Science 255*:989-991) and the KDR/FLK-1 receptor, discussed in the U.S. Patent Application No. 08/193,829. In addition, a receptor that binds αFGF and βFGF is identified. Jaye *et al.*, 1992, *Biochem. Biophys. Acta 1135*:185-199). Consequently, these receptor PTKs most likely regulate endothelial cell proliferation.

FGFRs play important roles in angiogenesis, wound healing, embryonic development, and malignant transformation. Basilico and Moscatelli, 1992, *Adv. Cancer Res. 59*:115-165. Four mammalian FGFR (FGFR1-4) have been described and additional diversity is generated by alternative RNA splicing within the extracellular domains. Jaye *et al.*, 1992, *Biochem. Biophys. Acta 1135*:185-199. Like other receptor PTKs, dimerization of FGF receptors is essential for their activation. Soluble or cell surface-bound heparin sulfate proteoglycans act in concert with FGF to induce dimerization (Schlessinger *et al.*, 1995, *Cell 83*:357-360), which leads to autophosphorylation of specific tyrosine residues in the cytoplasmic domain. Mohammadi et al., 1996, *Mol. Cell Biol. 16*:977-989.

Mutations in three human FGF receptor genes, FGFR1, FGFR2, and FGFR3, have been implicated in a variety of human genetic skeletal disorders. Mutations in FGFR1 and FGFR2 result in the premature fusion of the flat bones of the skull and cause the craniosynostosis syndromes, such as Apert (FGFR2) (Wilkie et al., 1994, *Nat. Genet. 8*:269-274), Pfeiffer (FGFR1 and FGFR2) (Muenke et al., 1994, Nat. Genet. 8:269-274), Jackson-Weiss (FGFR2) (Jabs et al., 1994, *Nat. Genet. 8*:275-279) and Crouzon (FGFR2) (Jabs et al., 1994, *Nat. Genet. 8*:275-279) syndromes. In contrast mutations in FGFR3 are implicated in long bone disorders and cause several clinically related forms of dwarfism including achondroplasia (Shiang et al., 1994, *Cell 78*:335-342), hypochondroplasia (Bellus et al., 1995, *Nat. Genet. 10*:357-359) and the neonatal lethal thanatophoric dysplasia (Tavormina et al., 1995, *Nat. Genet. 9*:321-328). It has been shown that these mutations lead to constitutive activation of the tyrosine kinase activity of FGFR3 (Webster et al., 1996, *EMBO J. 15*:520-527). Furthermore gene-targeting experiments in mice have revealed an essential role for FGFR3 in developmental bone formation (Deng et al., 1996, *Cell 84*:911-921).

Another major role proposed for FGFs *in vivo* is the induction of angiogenesis (Folkman and Klagsbrun, 1987, *Science 236*:442). Therefore, inappropriate expression of FGFs or of their receptors or aberrant function of the tyrosine kinase activity could contribute to several human angiogenic pathologies such as diabetic retinopathy, rheumatoid arthritis, atherosclerosis and tumor neovascularization (Klagsbrun and Edelman, 1989, *Arteriosclerosis 9*:269). Moreover, FGFs are thought to be involved in malignant transformation. Indeed, the genes coding for the three FGF homologues int-2, FGF-5 and hst-1/K-fgf were originally isolated as oncogenes. Furthermore, the cDNA encoding FGFR1 and FGFR2 are amplified in a population of breast cancers (Adnane et al., 1991, *Oncogene 6*:659-663). Over-expression of FGF receptors has been also detected in human pancreatic cancers, astrocytomas, salivary gland adenosarcomas, Kaposi sarcomas, ovarian cancers and prostate cancers.

Evidence, such as the disclosure set forth in copending U.S. Application Serial No. 08/193,829, strongly suggests that VEGF is not only responsible for endothelial cell proliferation, but also is a prime regulator of normal and pathological angiogenesis. *See generally*, Klagsburn and Soker, 1993, *Current Biology 3*:699-702; Houck *et al.*, 1992, *J. Biol. Chem. 267*:26031-26037. Moreover, it has been shown that KDR/FLK-1 and flt-1 are abundantly expressed in the proliferating endothelial cells of a growing tumor, but not in the surrounding quiescent endothelial cells. Plate *et al.*, 1992, *Nature 359*:845-848; Shweiki *et al.*, 1992, *Nature 359*:843-845.

The invention is directed to designing and identifying modulators of receptor and non-receptor PTK functions that could modify the inappropriate activity of a PTK involved with a clinical disorder. The rational design and identification of modulators of PTK functions can be accomplished by utilizing the structural coordinates that define a PTK three dimensional structure.

## II. Modulators of PTK functions as Therapeutics for Disease

As a consequence of the disorders discussed above, scientists in the biomedical community are searching for modulators of PTK functions that down-regulate signal transduction pathways associated with inappropriate PTK activity.

In particular, small molecule modulators of PTK functions are sought as some can traverse the cell membrane and do not hydrolyze in acidic environments. Some compounds have already been discovered. For example, bis monocyclic, bicyclic or heterocyclic aryl compounds (PCT WO 92/20642), vinylene-azaindole derivatives (PCT WO 94/14808) 1-cyclopropyl-4-pyridyl-quinolones (U.S. Patent No. 5,330,992), styryl compounds (U.S. Patent No. 5,217,999), styryl-substituted pyridyl compounds (U.S. Patent No. 5,302,606), certain quinazoline derivatives (EP Application No. 0 566 266 A1), seleoindoles and selenides (PCT WO 94/03427), tricyclic polyhydroxylic compounds (PCT WO 92/21660), and benzylphosphonic acid compounds (PCT WO 91/15495) are described as PTK inhibitors.

Although some modulators of PTK function are known, many of these are not specific for PTK subfamilies and will therefore cause multiple side-effects as therapeutics. Compounds of the oxindolinone/ thiolindolinone family, however, are specific for the FGF receptor subfamily (U.S. Patent Application Serial No. 08/702,232, filed August 23, 1996, invented by Tang et al., entitled "Indolinone Combinatorial Libraries and Related Products and Methods for the Treatment of

Disease," Attorney Docket No. 221/187). In addition, compounds of the oxindolinone/thiolindolinone family are non-hydrolyzable in acidic conditions and can be highly bioavailable.

The invention provides information regarding the specific interactions between a PTK and compounds of the oxindolinone/thiolindolinone family. Although the use of X-ray crystallography has provided three dimensional structures of other PTKs, the PTKs in these structures are not complexed with PTK subfamily specific, hydrolysis resistant, highly bioavailable small molecules. The X-ray crystallography techniques used in the current invention resolve interactions between a PTK and compounds in complex with it at the atomic level, which provides detailed information regarding the orientation of chemical groups defining an effective modulator of PTK function.

## III. Crystalline Tyrosine Kinases

Crystalline PTKs of the invention include native crystals, derivative crystals and co-crystals. The native crystals of the invention generally comprise substantially pure polypeptides corresponding to the tyrosine kinase domain in crystalline form.

It is to be understood that the crystalline tyrosine kinase domains of the invention are not limited to naturally occurring or native tyrosine kinase domains. Indeed, the crystals of the invention include mutants of native tyrosine kinase domains. Mutants of native tyrosine kinase domains are obtained by replacing at least one amino acid residue in a native tyrosine kinase domain with a different amino acid residue, or by adding or deleting amino acid residues within the native polypeptide or at the N- or C-terminus of the native polypeptide, and have substantially the same three-dimensional structure as the native tyrosine kinase domain from which the mutant is derived.

By having substantially the same three-dimensional structure is meant having a set of atomic structure coordinates that have a root-mean-square deviation of less than or equal to about 2Å when superimposed with the atomic structure coordinates of the native tyrosine kinase domain from which the mutant is derived when at least about 50% to 100% of the Cα atoms of the native tyrosine kinase domain are included in the superposition.

Amino acid substitutions, deletions and additions which do not significantly interfere with the three-dimensional structure of the tyrosine kinase domain will depend, in part, on the region of the tyrosine kinase domain where the substitution, addition or deletion occurs. In highly variable regions of the molecule, such as those shown in FIG. 6, non-conservative substitutions as well as conservative substitutions may be tolerated without significantly disrupting the three-dimensional structure of the molecule. In highly conserved regions, or regions containing significant secondary structure, such as those regions shown in FIG. 6, conservative amino acid substitutions are preferred.

Conservative amino acid substitutions are well-known in the art, and include substitutions made on the basis of similarity in polarity, charge, solubility, hydrophobicity, hydrophilicity and/or the amphipathic nature of the amino acid residues involved. For example, negatively charged amino acids include aspartic acid and glutamic acid; positively charged amino acids include lysine and arginine; amino acids with uncharged polar head groups having similar hydrophilicity values include the following: leucine, isoleucine, valine; glycine, alanine; asparagine, glutamine; serine, threonine; phenylalanine, tyrosine. Other conservative amino acid substitutions are well known in the art.

For tyrosine kinase domains obtained in whole or in part by chemical synthesis, the selection of amino acids available for substitution or addition is not limited to the genetically encoded amino acids. Indeed, the mutants described herein may contain non-genetically encoded amino acids. Conservative amino acid substitutions for many of the commonly known non-genetically encoded amino acids are well known in the art. Conservative substitutions for other amino acids can be determined based on their physical properties as compared to the properties of the genetically encoded amino acids.

In some instances, it may be particularly advantageous or convenient to substitute, delete and/or add amino acid residues to a native tyrosine kinase domain in order to provide convenient cloning sites in cDNA encoding the polypeptide, to aid in purification of the polypeptide, and for crystallization of the polypeptide. Such substitutions, deletions and/or additions which do not substantially alter the three dimensional structure of the native tyrosine kinase domain will be apparent to those of ordinary skill in the art.

It should be noted that the mutants contemplated herein need not exhibit PTK activity. Indeed, amino acid substitutions, additions or deletions that interfere with the kinase activity of the tyrosine kinase domain but which do not significantly alter the three-dimensional structure of the domain are specifically contemplated by the invention. Such crystalline polypeptides, or the atomic structure coordinates obtained therefrom, can be used to identify compounds that bind to the native domain. These compounds may affect the activity or the native domain.

The derivative crystals of the invention generally comprise a crystalline tyrosine kinase domain polypeptide in covalent association with one or more heavy metal atoms. The polypeptide may correspond to a native or a mutated tyrosine kinase domain. Heavy metal atoms useful for providing derivative crystals include, by way of example and not limitation, gold, mercury, etc.

The co-crystals of the invention generally comprise a crystalline tyrosine kinase domain polypeptide in association with one or more compounds. The association may be covalent or non-covalent. Such compounds include, but are not limited to, cofactors, substrates, substrate analogues, inhibitors, allosteric effectors, etc.

## IV. Three Dimensional Structure Determination Using X-ray Crystallography

X-ray crystallography is a method of solving the three dimensional structures of molecules. The structure of a molecule is calculated from X-ray diffraction patterns using a crystal as a diffraction grating. Three dimensional structures of protein molecules arise from crystals grown from a concentrated aqueous solution of that protein. The process of X-ray crystallography can include the following steps:

(a) synthesizing and isolating a polypeptide;

(b) growing a crystal from an aqueous solution comprising the polypeptide with or without a modulator; and

(c) collecting X-ray diffraction patterns from the crystals, determining unit cell dimensions and symmetry, determining electron density, fitting the amino acid sequence of the polypeptide to the electron density, and refining the structure.

### Production of Polypeptides

The native and mutated tyrosine kinase domain polypeptides described herein may be chemically synthesized in whole or part using techniques that are well-known in the art (see, e.g., Creighton, 1983). Alternatively, methods which are well known to those skilled in the art can be used to construct expression vectors containing the native or mutated tyrosine kinase domain polypeptide coding sequence and appropriate transcriptional/translational control signals. These methods include *in vitro* recombinant DNA techniques, synthetic techniques and *in vivo* recombination/genetic recombination. See, for example, the techniques described in Maniatis *et al.*, 1989 and Ausubel *et al.*, 1989.

A variety of host-expression vector systems may be utilized to express the tyrosine kinase domain coding sequence. These include but are not limited to microorganisms such as bacteria transformed with recombinant bacteriophage DNA, plasmid DNA or cosmid DNA expression vectors containing the tyrosine kinase domain coding sequence; yeast transformed with recombinant yeast expression vectors containing the tyrosine kinase domain coding sequence; insect cell systems infected with recombinant virus expression vectors (e.g., baculovirus) containing the tyrosine kinase domain coding sequence; plant cell systems infected with recombinant virus expression vectors (e.g., cauliflower mosaic virus, CaMV; tobacco mosaic virus, TMV) or transformed with recombinant plasmid expression vectors (e.g., Ti plasmid) containing the tyrosine kinase domain coding sequence; or animal cell systems. The expression elements of these systems vary in their strength and specificities.

Depending on the host/vector system utilized, any of a number of suitable transcription and translation elements, including constitutive and inducible promoters, may be used in the expression vector. For example, when cloning in bacterial systems, inducible promoters such as pL of bacteriophage λ, plac, ptrp, ptac (ptrp-lac hybrid promoter) and the like may be used; when cloning in insect cell systems, promoters such as the baculovirus polyhedrin promoter may be used; when cloning in plant cell systems, promoters derived from the genome of plant cells (e.g., heat shock promoters; the promoter for the small subunit of RUBISCO; the promoter for the chlorophyll a/b binding protein) or from plant viruses (e.g., the 35S RNA promoter of CaMV; the coat protein promoter of TMV) may be used; when cloning in mammalian cell systems, promoters derived from the genome of mammalian cells (e.g., metallothionein promoter) or from mammalian viruses (e.g., the adenovirus late promoter; the vaccinia virus 7.5K promoter) may be used; when generating cell lines that contain multiple copies of the tyrosine kinase domain DNA, SV40-, BPV- and EBV-based vectors may be used with an appropriate selectable marker.

Methods describing methods of DNA manipulation, vectors, various types of cells used, methods of incorporating the vectors into the cells, expression techniques, protein purification and isolation methods, and protein concentration methods are disclosed in detail with respect to the protein PYK-2 in PCT publication WO 96/18738. This publication is incorporated herein by reference in its entirety, including any drawings. Those skilled in the art will appreciate that such descriptions are applicable to the present invention and can be easily adapted to it.

Crystal Growth

Crystals are grown from an aqueous solution containing the purified and concentrated polypeptide by a variety of techniques. These techniques include batch, liquid, bridge, dialysis, vapor diffusion, and hanging drop methods. McPherson, 1982, John Wiley, New York; McPherson, 1990, *Eur. J. Biochem. 189*:1-23; Webber, 1991, *Adv. Protein Chem. 41*:1-36, incorporated by reference herein in its entirety, including all figures, tables, and drawings.

Generally, the native crystals of the invention are grown by adding precipitants to the concentrated solution of the polypeptide corresponding to the PTK catalytic domain. The precipitants are added at a concentration just below that necessary to precipitate the protein. Water is removed by controlled evaporation to produce precipitating conditions, which are maintained until crystal growth ceases.

For crystals of the invention, it has been found that hanging drops containing about 2.0 $\mu$L of tyrosine kinase domain polypeptide (10 mg/mL in 10mM Tris-HCl, pH 8.0, 10 mM NaCl and 2 mM dithiothreitol) and 2.0 $\mu$L reservoir solution (16% w/v polyethylene glycol MW 10000, 0.3 M $(NH_4)_2SO_4$, 5% v/v ethylene glycol or glycerol and 100 mM bis-Tris, pH 6.5) suspended over 0.5 mL reservoir buffer for about 3-4 weeks at 4°C provide crystals suitable for high resolution X-ray structure determination.

Those of ordinary skill in the art will recognize that the above-described crystallization conditions can be varied. Such variations may be used alone or in combination, and include polypeptide solutions containing polypeptide concentrations between about 1 mg/mL and about 60 mg/mL, Tris-HCl concentrations between about 10 mM and about 200 mM, dithiothreitol concentrations between about 0 mM and about 20 mM, pH ranges between about 5.5 and about 7.5; and reservoir solutions containing polyethylene glycol concentrations between about 10% and about 30% (w/v), polyethylene glycol molecular weights between about 1000 and about 20,000, $(NH_4)_2SO_4$ concentrations between about 0.1 M and about 0.5 M, ethylene glycol or glycerol concentrations between about 0% and about 20% (v/v), bis-Tris concentrations between about 10 mM and about 200 mM, pH ranges between about 5.5 and about 7.5 and temperature ranges between about 0° C and about 25°C. Other buffer solutions may be used such as HEPES buffer, so long as the desired pH range is maintained.

Derivative crystals of the invention can be obtained by soaking native crystals in mother liquor containing salts of heavy metal atoms. It has been found that soaking a native crystal in a solution containing about 0.1 mM to about 5 mM thimerosal, 4-chloromeruribenzoic acid or $KAu(CN)_2$ for about 2 hr to about 72 hr provides derivative crystals suitable for use as isomorphous replacements in determining the X-ray crystal structure of the tyrosine kinase domain polypeptide.

Co-crystals of the invention can be obtained by soaking a native crystal in mother liquor containing compound that bind the kinase domain, or described above, or can be obtained by co-crystallizing the kinase domain polypeptide in the presence of one or more binding compounds.

For co-crystals of tyrosine kinase domain polypeptide in co-complex with AMP-PCP, it has been found that co-crystallizing the kinase domain polypeptide in the presence of AMP-PCP using the above-described crystallization conditions for obtaining native crystals with a polypeptide solution additionally containing 10 mM AMP-PCP and 20 mM $MgCl_2$ yields co-crystals suitable for the high resolution structure determination by X-ray crystallography. Of course, those having skill in the art will recognize that the concentrations of AMP-PCP and $MgCl_2$ in the polypeptide solution can be varied, alone or in combination with the variations described above for native crystals. Such variations include polypeptide solutions containing AMP-PCP concentrations between 0.1 mM and 50 mM and $MgCl_2$ concentrations between 0 mM and 50 mM.

Crystals comprising a polypeptide corresponding to a PTK catalytic domain complexed with a compound can be grown by one of two methods. In the first method, the modulator is added to the aqueous solution containing the polypeptide corresponding to the PTK catalytic domain before the crystal is grown. In the second method, the modulator is soaked into an already existing crystal of a polypeptide corresponding to a PTK catalytic domain.

Crystalline FGFR

In one illustrative embodiment, the invention provides crystals of FGFR1. The crystals were obtained by the methods provided in the Examples. The FGFR1 crystals, which may be native crystals, derivative crystals or co-crystals, have monoclinic unit cells (i.e., unit cells wherein $a \neq b \neq c$; $\alpha = \gamma = 90°$; and $\beta > 90°$) and space group symmetry C2. There are two FGFR1 molecules in the asymmetric unit, related by an approximate two-fold axis.

Two forms of crystalline FGFR1 were obtained. In one form (designated "C2-A form"), the unit cell has dimensions of a=208.3 Å, b=57.2 Å, c=65.5 Å and β=107.2°. In another form (designated "C2-B form"), the unit cell has dimensions of a=211.6 Å, b=51.3 Å, c=66.1 Å and β=107.7°.

Three distinct two-fold related FGFR1 dimers are observed in both the C2-A and C2-B forms of the FGFR1 crystal, one non-crystallographically related dimer and two crystallographically related dimers. The non-crystallographically related dimer comprises the two molecules in the asymmetric unit. The residues making up the dimer interface are located in C-terminal lobe. In this dimer, the C-terminal lobes abut with the N-terminal lobes distal to one another. The total amount of surface area buried in the surface is about 950 $Å^2$. Very few of the interactions in the interface are of a specific nature, e.g., hydrogen-bonding or close packing of hydrophobic residues.

There are two crystallographically-related dimers in the C2 lattice. In the first dimer, the residues that constitute the dimer interface are limited to those in the β-sheet of the N-terminal lobe (amino acid residues 477, 479, 498, 506, 508 and 496). The total surface area buried in this interface is about 670 Å². The interactions are rather specific. Three hydrophobic residues which are partially solvent-exposed in the monomer, Val-479, Ile-498 and Val-508, come together with their two-fold-related residues to form a compact hydrophobic plug. This plug is capped on either side by a salt bridge between Arg-477 and Glu-496. In addition, two main-chain hydrogen-bonds connect the β-sheets of the two monomers at the start of β3 (amino acid residues 506 and 508). The residues in this dimer interface, or their residue character, are generally conserved in the mammalian FGF receptors, but not in the invertebrate homologues.

The other crystallographically-related dimer buries about 1650 Å² in its interface. In this dimer, the αC helices of the two monomers are nearly parallel and contact each other at their C-terminal ends. Met-534 and Met-537 are in van der Waals contact with their two-fold-related residues. Other hydrophobic contacts involve Pro-466 with Ile-648 and Pro-469 with Ile-676 and Thr-678. In addition, hydrogen bonds (side-chain to main-chain) are made between Arg-470 and Lys-618 and between His-649 and Glu-464, and there are several water molecules that bridge the two monomers through hydrogen bonding.

In the C2-B form of the crystal, the monomers of this second crystallographically-related dimer are shifted slightly with respect to one another (6°

rotation), indicating that this interface is somewhat fluid.

In both of the crystallographically-related dimers, the N-termini of the two molecules comprising the dimer point in the same direction and are reasonably close to one another.

## Determining Unit Cell Dimensions and the Three Dimensional Structure of a Polypeptide or Polypeptide Complex

Once the crystal is grown, it can be placed in a glass capillary tube and mounted onto a holding device connected to an X-ray generator and an X-ray detection device. Collection of X-ray diffraction patterns are well documented by those in the art. Ducruix and Geige, 1992, IRL Press, Oxford, England, and references cited therein. A beam of X-rays enter the crystal and then diffract from the crystal. An X-ray detection device can be utilized to record the diffraction patterns emanating from the crystal. Although the X-ray detection device on older models of these instruments is a piece of film, modern instruments digitally record X-ray diffraction scattering.

Methods for obtaining the three dimensional structure of the crystalline form of a peptide molecule or molecule complex are well known in the art. Ducruix and Geige, 1992, IRL Press, Oxford, England, and references cited therein. The following are steps in the process of determining the three dimensional structure of a molecule or complex from X-ray diffraction data.

After the X-ray diffraction patterns are collected from the crystal, the unit cell dimensions and orientation in the crystal can be determined. They can be determined from the spacing between the diffraction emissions as well as the patterns made from these emissions. The unit cell dimensions are characterized in three dimensions in units of Angstroms (one Å = $10^{-10}$ meters) and by angles at each vertices. The symmetry of the unit cell in the crystals is also characterized at this stage. The symmetry of the unit cell in the crystal simplifies the complexity of the collected data by identifying repeating patterns. Application of the symmetry and dimensions of the unit cell is described below.

Each diffraction pattern emission is characterized as a vector and the data collected at this stage of the method determines the amplitude of each vector. The phases of the vectors can be determined using multiple techniques. In one method, heavy atoms can be soaked into a crystal, a method called isomorphous replacement, and the phases of the vectors can be determined by using these heavy atoms as reference points in the X-ray analysis. Otwinowski, 1991, Daresbury, United Kingdom, 80-86. The isomorphous replacement method usually requires more than one heavy atom derivative. In another method, the amplitudes and phases of vectors from a crystalline polypeptide with an already determined structure can be applied to the amplitudes of the vectors from a crystalline polypeptide of unknown structure and consequently determine the phases of these vectors. This second method is known as molecular replacement and the protein structure which is used as a reference must have a closely related structure to the protein of interest. Naraza, 1994, *Proteins 11*:281-296. Thus, the vector information from a PTK of known structure, such as those reported herein, are useful for the molecular replacement analysis of another PTK with unknown structure.

Once the phases of the vectors describing the unit cell of a crystal are determined, the vector amplitudes and phases, unit cell dimensions, and unit cell symmetry can be used as terms in a Fourier transform function. The Fourier transform function calculates the electron density in the unit cell from these measurements. The electron density that describes one of the molecules or one of the molecule complexes in the unit cell can be referred to as an electron density map. The amino acid structures of the sequence or the molecular structures of compounds complexed with the crystalline polypeptide may then fit to the electron density using a variety of computer programs. This step of the process is sometimes referred to as model building and can be accomplished by using computer programs such as TOM/FRODO. Jones, 1985, *Methods in Enzymology 115*:157-171.

A theoretical electron density map can then be calculated from the amino acid structures fit to the experimentally determined electron density. The theoretical and experimental electron density maps can be compared to one another and the agreement between these two maps can be described by a parameter called an R-factor. A low value for an R-factor describes a high degree of overlapping electron density between a theoretical and experimental electron density map.

The *R*-factor is then minimized by using computer programs that refine the theoretical electron density map. A computer program such as X-PLOR can be used for model refinement by those skilled in the art. Brünger, 1992, *Nature* 355:472-475. Refinement may be achieved in an iterative process. A first step can entail altering the conformation of atoms defined in an electron density map. The conformations of the atoms can be altered by simulating a rise in temperature which will increase the vibrational frequency of the bonds and modify positions of atoms in the structure. At a particular point in the atomic perturbation process, a force field, which typically defines interactions between atoms in terms of allowed bond angles and bond lengths, Van der Waals interactions, hydrogen bonds, ionic interactions, and hydrophobic interactions, can be applied to the system of atoms. Favorable interactions may be described in terms of free energy and the atoms can be moved over many iterations until a free energy minimum is achieved. The refinement process can be iterated until the R-factor reaches a minimum value.

The three dimensional structure of the molecule or molecule complex is described by atoms that fit the theoretical electron density characterized by a minimum R-value. A file can then be created for the three dimensional structure that defines each atom by coordinates in three dimensions. Examples of such structural coordinate files are defined in Table 1, Table 2, Table 3, and Table 4.

## V. Structures of FGFR1

The present invention provides high-resolution three-dimensional structures and atomic structure coordinates of crystalline FGFR1 and crystalline FGFR1:AMP-PCP co-complex as determined by X-ray crystallography. The specific methods used to obtain the structure coordinates are provided in the examples. The atomic structure coordinates of crystalline FGFR1, obtained from the C2-A form of the crystal to 2.0 Å resolution, are listed in Table 3; the coordinates of crystalline FGFR1:AMP-PCP co-complex, obtained from the C2-A form of the crystal to 2.3 Å resolution are listed in Table 4.

Those having skill in the art will recognize that atomic structure coordinates as determined by X-ray crystallography are not without error. Thus, it is to be understood that any set of structure coordinates obtained for crystals of FGFR1, whether native crystals, derivative crystals or co-crystals, that have a root mean square deviation ("r.m.s.d.") of less than or equal to about 1.5 Å when superimposed, using backbone atoms (N, $C_\alpha$, C and O), on the structure coordinates listed in Table 3 or Table 4 are considered to be identical with the structure coordinates listed in the Tables when at least about 50% to 100% of the backbone atoms of FGFR1 are included in the superposition.

Referring now to FIG. 1, the overall structure of FGFR1 is bi-lobate. The N-terminal lobe of FGFR1 spans amino acid residues 456-567 (FIG. 3) and comprises a curled β-sheet of five anti-parallel strands (β1-β5) and one α-helix (αC). The C-terminal lobe spans amino acid residues 568-765 (FIG. 3) and comprises two β-strands (β7, β8) and seven α-helices (αD, αE, αEF, αF-αI). The secondary structure nomenclature follows that used for IRK (Hubbard *et al.*, 1994) which in turn is based on the assignments for cAPK (Knighton *et al.*, 1991). FIG. 2 shows a stereo view of a $C_\alpha$ trace of FGFR1 in the same orientation as FIG. 1.

A structure-based sequence alignment of the tyrosine kinase domains of human fibroblast growth factor receptor 1 (human FGFR1; labelled FGFR1), human fibroblast growth factor receptors 2, 3 and 4 (labelled FGFR2, FGFR3 and FGFR4, respectively), a *D. melanogaster* homologue (labelled DFDFR1), a *C elegans* homologue (labelled EGL-15) and insulin receptor kinase (labelled IRK), is shown in FIG. 3. The sequence of FGFR1, which is not shown in FIG. 3 is identical to the sequence of FGFR1 except that FGFR1 has the following amino acid substitutions and additions: Cys-488 → Ala, Cys-584 → Ser, Leu-457 → Val and an additional five N-terminal amino acids (Ser-Ala-Ala-Gly-Thr). The secondary structure assignments for FGFR1 and IRK were obtained using the Kabsch and Sander algorithm (Kabsch and Sander, 1983) as implemented in PROCHECK (Laskowski *et al.*, 1993). In the FGF receptor sequences, a period represents sequence identity to FGFR1. In the IRK sequence, residues that are identical to FGFR1 are highlighted. A hyphen denotes an insertion.

The numbers under the EGL-15 sequence represent the fractional solvent accessibility (FSA2) of the residue in the FGFR1 structure. The FSA ratio is the ratio of the solvent-accessible surface area of a residue in a Gly-X-Gly tripeptide compared to that in the FGFR1 structure. A value of 0 represents an FSA between 0.00 and 0.09; 1 represents an FSA between 0.10 and 0.19, etc. The higher the value, the more solvent-exposed the residue. An asterisk or pound sign in the FSA line indicates that the residue (asterisk) or side chain (pound sign) is not included in the atom model due to disorder. The numbers below the FSA line are the FSAs for those residues that form part of a dimer interface.

The amino acid residue numbers for FGFR1, and hence FGFR1, and IRK provided in FIG. 3 are used in the discussion that follows. Significant differences in the N-terminal lobe of FGFR1 as compared to IRK are found in the loops between β strands and in αC. Residues from the end of β1 through the beginning of β2 (amino acid residues 485-490) form the nucleotide-binding loop, named because of its role in ATP coordination. This residue stretch contains the protein kinase-conserved GXGXXG sequence motif, where X is any amino acid. This loop is poorly ordered in one FGFR1 molecule in the asymmetric unit and disordered (i.e., not included in the atomic model) in the other FGFR1 molecule in the asymmetric unit. The loop between β1 and β3 is disordered in both FGFR1 molecules comprising the asymmetric unit.

Referring now to FIG. 4A, which provides a ribbon diagram of the N-terminal lobes of FGFR1 and IRK in which the $C_\alpha$ atoms of the β-sheets have been superimposed, it can be seen that in FGFR1 αC is longer by one helical turn than in IRK and is oriented such that residues Lys-514 and Glu-531, which are conserved in protein kinases, form a salt bridge (represented by a black line). While not intending to be bound by theory, this salt bridge is believed to be important for proper positioning of the conserved lysine side chain, which coordinates two phosphate oxygens of ATP. The salt bridge is observed in the structures of cAPK (Knighton *et al.*, 1991) and mitogen-activated protein kinase (MAPK) (Zhang *et al.*, 1994).

Referring now to FIG. 4B, which provides a ribbon diagram of the C-terminal lobes of FGFR1 and IRK in which the $C_\alpha$ atoms of the α-helices have been superimposed, a significant difference is found in the C-terminal helix of FGFR1 when compared to IRK; helix αI of FGFR1 is longer by seven residues (two helical turns) than its counterpart in IRK. The extended length of αI is presumably important in the biological functioning of FGF receptors, since the tyrosine autophosphorylation site to which an SH2 domain of PLCγ binds is six residues C-terminal to this helix.

The structure of FGFR1 displays an open disposition of the N- and C-terminal lobes. Despite having different sets of lattice contacts, the two FGFR1 molecules in the asymmetric unit have only a 2° difference in relative lobe orientation. It appears as though the stearic interaction between residues in αC (Glu-531 and Met-534) with Phe-642 and Gly-643 of the protein kinase-conserved DFG sequence at the beginning of the activation loop accounts for the open conformation of FGFR1.

The active site of FGFR1 is characterized by at least amino acid residues spanning the catalytic loop, activation loop and nucleotide binding loop. Unlike the structure of IRK, in which Tyr-1162 occupies the active site of the molecule, the active sites of both FGFR1 molecules in the asymmetric unit are unoccupied.

The activation loop, which regulates phosphorylation, is characterized by at least resides 640 to 663. Quite surprisingly, while the activation loops of FGFR1 and IRK contain the same number of amino acid residues and share greater than 50% sequence homology, the paths of the polypeptide chains are strikingly dissimilar, diverging at Ala-640 (Gly-1149 in IRK) and reconverging at Val-664 (Val-1173 in IRK). Tyr-653 and Tyr 564 are not bound in the active site. Instead, these residues point away from it. Tyr-653 is in van der Waals contact with several hydrophobic residues (Val-664, Leu-672 and Phe-710) and is hydrogen-bonded via its hydroxyl group to a backbone carbonyl oxygen (Leu-672). Tyr-654 is more solvent exposed than Tyr-653, and its only van der Waals contact is with Val-706. Temperature factor data suggest that the activation loop is relatively mobile and adopts multiple conformations.

The catalytic loop of protein kinases lies between secondary structure elements αE and β7 and contains an invariant aspartic acid residue (Asp-623 in FGFR1) which serves as the catalytic base in the phosphotransfer reaction, abstracting the proton from the hydroxyl group of the substrate tyrosine, serine or threonine. The catalytic loop sequence of FGFR1 comprises at least residues His-621 to Asn-628 (amino acid sequence

HRDLAARN), and is identical to that for IRK and most receptor and non-receptor PTKs.

In addition to the two tyrosine autophosphorylation sites in the activation loop (Tyr-653 and Tyr-654), there are four other autophosphorylation sites present in the FGFR1 crystals of the invention: one in the juxtamembrane region (Tyr-463), two in the kinase insert (Tyr-583 and Tyr-585) and one in the C-terminal lobe (Tyr-730) (Mohammadi *et al.*, 1996). They exhibit varying degrees of conservation in mammalian FGF receptors: Tyr-463 and Tyr-585 in FGFR1 and 2; Tyr-583 in FGFR1, 2 and 3; and Tyr-730 in FGFR 1, 2, 3 and 4 (FIG. 3).

Referring now to FIG. 5, the positions of the autophosphorylation sites are mapped onto the FGFR1 structure. The juxtamembrane site (Tyr-463) and the residues N-terminal to it are disordered in one of the FGFR1 molecules in the asymmetric unit. In the other molecule in the asymmetric unit Tyr-463 is involved in a lattice contact.

The kinase insert region (the region between helices αD and αE) contains autophosphorylation sites Tyr-583 and Tyr-585 and is disordered in both FGFR1 molecules in the asymmetric unit of the C2-A form of the crystal. In the C2-B form, several lattice contacts partially pin down this region in one of the two FGFR1 molecules in the asymmetric unit, allowing a trace of the polypeptide chain to be made. There is no well-defined secondary structure for these residues. Tyr-730, situated in αH in the C-terminal lobe, is nearly buried and the side-chain hydroxyl group makes two hydrogen-bonds. The side chains of neighboring Met-732 and Met-733 are both buried. Therefore, phosphorylation of Tyr-730 would presumably require prior unfolding of αH.

Aside from Tyr-730, the five other autophosphorylation sites (including Tyr-653 and Tyr-654) are found in relatively mobile segments of the FGFR1 molecule. While not intending to be bound by theory, the spatial positions of the autophosphorylation sites relative to the active site suggest that autophosphorylation occurs by a *trans* mechanism between two kinase domains, supporting the hypothesis that ligand-induced receptor dimerization is critical for the initiation of autophosphorylation events.

The structure of crystalline FGFR1:AMP-PCP co-complex is essentially similar to that observed for crystalline FGFR1. There are no significant changes in the structure of FGFR1 induced by AMP-PCP binding. In particular, binding of AMP-PCP, and by extension ATP, does not by itself promote lobe closure under the crystallization conditions used. Furthermore, complexation did not result in any noticeable changes in the conformations of the activation and nucleotide-binding loops.

The crystalline FGFR1:AMP-PCP co-complex contains hydrogen bonds that are present between N1 of adenine and the amide nitrogen of Ala-564 and between N6 of adenine and the carbonyl oxygen of Glu-562. The adenine ring is flanked on one side by Leu-484 and Val-492 (N-terminal lobe) and on the other side by Leu-630 (C-terminal lobe). The ribose hydroxyl groups make no direct hydrogen bonds with protein atoms. Lys-514 is hydrogen-bonded to oxygens of the β- and γ-phosphates. There is no unambiguous electron density that would indicate the positions of $Mg^{2+}$ ions. Generally, AMP-PCP appears to be coordinated rather loosely to unphosphorylated FGFR1, being bound to the "roof" of the cleft rather than being tightly sandwiched between the two kinase lobes.

## Structural Differences Between FGF-R and IRK

Several features distinguish the FGF-receptor structure from that of the insulin-receptor tyrosine kinase. These distinctions are likely to be important in signaling by FGF-receptors, and other monomeric receptors that are believed to undergo ligand-induced dimerization.

The most significant difference between the structures of FGFR1 and IRK is the conformation of the activation loop. In FGFR1, the activation loop is disposed such that the binding site for substrate peptides is blocked not by an activation loop tyrosine, as in IRK, but by Arg-661 and PTK-invariant Pro-663, while the ATP binding site is accessible. This represents another molecular mechanism by which a receptor PTK may be autoinhibited. The observed autoinhibition in FGFR1 would appear to be weaker than that in IRK because of fewer specific interactions made by residues in the FGFR1 activation loop (manifested in the relatively higher B-values) and the accessibility of the ATP site. One obvious distinction between the insulin and FGF receptor families is that in the former, receptors are covalently linked heterotetramers ($\alpha_2\beta_2$), whereas in the latter, receptor dimerization is ligand dependent. Receptors whose kinase domains are always in close proximity may require a stronger autoinhibition mechanism than those receptors that associate only upon ligand binding (Taylor *et al.*, 1995). Since most growth factor receptors undergo ligand-dependent dimerization and activation, the FGF receptor autoinhibition mechanism appears to be a more general one.

## VI. Uses of the Crystals and Atomic Structure Coordinates

The crystals of the invention, and particularly the atomic structure coordinates obtained therefrom, have a wide variety of uses. For example, the crystals described herein can be used as a starting material in any of the art-known methods of use for receptor and non-receptor tyrosine kinases. Such methods of use include, for example, identifying molecules that bind to the native or mutated catalytic domain of tyrosine kinases. The crystals and structure coordinates are particularly useful for identifying compounds that inhibit receptor and non-receptor tyrosine kinases as an approach towards developing new therapeutic agents (see, e.g., Levitzki and Gazit, 1995).

The structure coordinates described herein can be used as phasing models for determining the crystal structures of additional native or mutated tyrosine kinase domains, as well as the structures of co-crystals of such domains with ligands such as inhibitors, agonists, antagonists, and other molecules. The structure coordinates, as well as models of the three-dimensional structures obtained therefrom, can also be used to aid the elucidation of solution-based structures of native or mutated tyrosine kinase domains, such as those obtained via NMR. Thus, the crystals and atomic structure coordinates of the invention provide a convenient means for elucidating the structures and functions of receptor and non-receptor tyrosine kinases.

For purposes of clarity and discussion, the crystals of the invention will be described by reference to specific FGFR1 exemplary crystals. Those skilled in the art will appreciate that the principles described herein are generally applicable to crystals of the tyrosine kinase domain of any cytoplasmic tyrosine kinase that undergoes ligand-induced dimerization or receptor tyrosine kinase, including but not limited to the tyrosine kinases of FIG. 6.

## VII. Structure Determination for PTKs with Unknown Structure Using Structural Coordinates

Structural coordinates, such as those set forth in Table 1, Table 2, Table 3, and Table 4, can be used to determine the three dimensional structures of PTKs with unknown structure. The methods described below can apply structural coordinates of a polypeptide with known structure to another data set, such as an amino acid sequence, X-ray crystallographic diffraction data, or nuclear magnetic resonance (NMR) data. Preferred embodiments of the invention relate to determining the three dimensional structures of PTKs and related polypeptides. These include receptor PTKs such as FGF-

R, PDGF-R, KDR, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK. Non-receptor PTKs such as SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK can also be used in the methods described herein.

## Structures Using Amino Acid Homology

Homology modeling is a method of applying structural coordinates of a polypeptide of known structure to the amino acid sequence of a polypeptide of unknown structure. This method is accomplished using a computer representation of the three dimensional structure of a polypeptide or polypeptide complex, the computer representation of amino acid sequences of the polypeptides with known and unknown structures, and standard computer representations of the structures of amino acids. Homology modeling comprises the steps of (a) aligning the amino acid sequences of the polypeptides with and without known structure; (b) transferring the coordinates of the conserved amino acids in the known structure to the corresponding amino acids of the polypeptide of unknown structure; refining the subsequent three dimensional structure; and (d) constructing structures of the rest of the polypeptide. One skilled in the art recognizes that conserved amino acids between two proteins can be determined from the sequence alignment step in step (a).

The above method is well known to those skilled in the art. Greer, 1985, *Science 228*, 1055. Blundell *et al.*, 1988, *Eur. J. Biochem. 172*, 513. A computer program currently utilized for homology modeling by those skilled in the art is the Homology module in the Insight II modeling package distributed by Molecular Simulations Inc.

Alignment of the amino acid sequence is accomplished by first placing the computer representation of the amino acid sequence of a polypeptide with known structure above the amino acid sequence of the polypeptide of unknown structure. Amino acids in the sequences are then compared and groups of amino acids that are homologous (*e.g.*, amino acid side chains that are similar in chemical nature - aliphatic, aromatic, polar, or charged) are grouped together. This method will detect conserved regions of the polypeptides and account for amino acid insertions or deletions.

Once the amino acid sequences of the polypeptides with known and unknown structures are aligned, the structures of the conserved amino acids in the computer representation of the polypeptide with known structure are transferred to the corresponding amino acids of the polypeptide whose structure is unknown. For example, a tyrosine in the amino acid sequence of known structure may be replaced by a phenylalanine, the corresponding homologous amino acid in the amino acid sequence of unknown structure.

The structures of amino acids located in non-conserved regions are to be assigned manually by either using standard peptide geometries or molecular simulation techniques, such as molecular dynamics. The final step in the process is accomplished by refining the entire structure using molecular dynamics and/or energy minimization.

The homology modeling method is well known to those skilled in the art and has been practiced using different protein molecules. The three dimensional structure of the polypeptide corresponding to the catalytic domain of a serine/threonine protein kinase, myosin light chain protein kinase, was homology modeled from the cAMP-dependent protein kinase catalytic subunit. Knighton *et al.*, 1992, *Science* *258*:130-135.

Structures Using Molecular Replacement

Molecular replacement is a method of applying the X-ray diffraction data of a polypeptide of known structure to the X-ray diffraction data of a polypeptide of unknown sequence. This method can be utilized to define the phases describing the X-ray diffraction data of a polypeptide of unknown structure when only the amplitudes are known. X-PLOR is a commonly utilized computer software package used for molecular replacement. Brünger, 1992, *Nature* 355:472-475. AMORE is another program used for molecular replacement. Navaza, 1994, *Acta Crystallogr.* A50:157-163. Preferably, the resulting structure does not exhibit a root-mean-square deviation of more than 3 Å.

A goal of molecular replacement is to align the positions of atoms in the unit cell by matching electron diffraction data from two crystals. A program such as X-PLOR can involve four steps. A first step can be to determine the number of molecules in the unit cell and define the angles between them. A second step can involve rotating the diffraction data to define the orientation of the molecules in the unit cell. A third step can be to translate the electron density in three dimensions to correctly position the molecules in the unit cell. Once the amplitudes and phases of the X-ray diffraction data is determined, an *R*-factor can be calculated by comparing electron diffraction maps calculated experimentally from the reference data set and calculated from the new data set. An R-factor between 30-50% indicates that the orientations of the atoms in the unit cell are reasonably determined by this method. A fourth step in the process can be to decrease the R-factor to roughly 20% by refining the new electron density map using iterative refinement techniques described herein and known to those or ordinary skill in the art.

Structures Using NMR Data

Structural coordinates of a polypeptide or polypeptide complex derived from X-ray crystallographic techniques can be applied towards the elucidation of three dimensional structures of polypeptides from nuclear magnetic resonance (NMR) data. This method is used by those skilled in the art. Wuthrich, 1986, John Wiley and Sons, New York:176-199; Pflugrath *et al.*, 1986, *J. Molecular Biology 189*:383-386; Kline *et al.*, 1986, *J. Molecular Biology 189*:377-382. While the secondary structure of a polypeptide is often readily determined by utilizing two-dimensional NMR data, the spatial connections between individual pieces of secondary structure are not as readily determinable. The coordinates defining a three-dimensional structure of a polypeptide derived from X-ray crystallographic techniques can guide the NMR spectroscopist to an understanding of these spatial interactions between secondary structural elements in a polypeptide of related structure.

The knowledge of spatial interactions between secondary structural elements can greatly simplify Nuclear Overhauser Effect (NOE) data from two-dimensional NMR experiments. Additionally, applying the crystallographic coordinates after the determination of secondary structure by NMR techniques only simplifies the assignment of NOEs relating to particular amino acids in the polypeptide sequence and does not greatly bias the NMR analysis of polypeptide structure. Conversely, using the crystallographic coordinates to simplify NOE data while determining secondary structure of the polypeptide would bias the NMR analysis of protein structure.

As the analysis of polypeptide structure by NMR methods is a relatively new technique, the use of structural coordinates defining a PTK structure will most likely be utilized more frequently in the near future. As the method progresses, the three dimensional structure analysis of polypeptides of the same size as a PTK catalytic domain will become more frequent.

## VIII. Structure-Based Design of Modulators of PTK Function Utilizing Structural Coordinates

Structure-based modulator design and identification methods are powerful techniques that can involve searches of computer data bases containing a wide variety of potential modulators and chemical functional groups. The computerized design and identification of modulators is useful as the computer data bases contain more compounds than the chemical libraries, often by an order of magnitude. For reviews of structure-based drug design and identification *see* Kuntz *et al.*, 1994, *Acc. Chem. Res. 27*:117; Guida, 1994, *Current Opinion in Struc. Biol. 4*: 777; Colman, 1994, *Current Opinion in Struc. Biol. 4*: 868.

The three dimensional structure of a polypeptide defined by structural coordinates can be utilized by these design methods. The structural coordinates of Table 1, Table 2, Table 3, and Table 4 can be utilized by this method. In addition, the three dimensional structures of receptor and non-receptor PTKs determined by the homology, molecular replacement, and NMR techniques described herein can also be applied to modulator design and identification methods. Thus, the structures of receptor PTKs, FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK, can be utilized by the methods described herein. The structures of non-receptor PTKs, SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK, can also be utilized by the rational modulator design method.

<u>Design by Searching Molecular Data Bases</u>

One method of rational modulator design searches for modulators by docking the computer representation of compounds from a data base of molecules. Publicly available data bases include:

a) ACD from Molecular Designs Limited

b) NCI from National Cancer Institute
c) CCDC from Cambridge Crystallographic Data Center
d) CAST from Chemical Abstract Service
e) Derwent from Derwent Information Limited
f) Maybridge from Maybridge Chemical Company LTD
g) Aldrich from Aldrich Chemical Company
h) Directory of Natural Products from Chapman & Hall

One such data base (ACD distributed by Molecular Designs Limited Information Systems) contains, for example, 200,000 compounds that are synthetically derived or are natural products. Methods available to those skilled in the art can convert a data set represented in two dimensions to one represented in three dimensions. These methods are enabled by such computer programs as CONCORD from Tripos Associates or DB-Converter from Molecular Simulations Limited.

Multiple methods of structure-based modulator design are known to those in the art. Kuntz *et al.*, 1982, *J. Mol. Biol. 162*: 269; Kuntz *et al.*, 1994, *Acc. Chem. Res. 27*: 117; Meng *et al.*, 1992, *J. Compt. Chem. 13*: 505; Bohm, 1994, *J. Comp. Aided Molec. Design 8*: 623.

A computer program widely utilized by those skilled in the art of rational modulator design is DOCK from the University of California in San Francisco. The general methods utilized by this computer program and programs like it are described in three applications below. More detailed information regarding some of these techniques can be found in the Molecular Simulations User Guide, 1995.

A typical computer program used for this purpose can comprise the following steps:

(a) remove the existing compound from the protein;

(b) dock the structure of another compound into the active-site using the computer program (such as DOCK) or by interactively moving the compound into the active-site;

(c) characterize the space between the compound and the active-site atoms;

(d) search libraries for molecular fragments which (i)can fit into the empty space between the compound and the active-site, and (ii) can be linked to the compound; and

(e) link the fragments found above to the compound and evaluate the new modified compound.

Part (c) refers to characterizing the geometry and the complementary interactions formed between the atoms of the active-site and the compounds. A favorable geometric fit is attained when a significant surface area is shared between the compound and active-site atoms without forming unfavorable steric interactions.

One skilled in the art would note that the method can be performed by skipping parts (d) and (e) and screening a data base of many compounds.

Structure-based design and identification of modulators of PTK function can be used in conjunction with assay screening. As large computer data base of compounds (around 10,000 compounds) can be searched in a matter of hours, the computer based method can narrow the compounds tested as potential modulators of PTK function in cellular assays.

The above descriptions of structure-based modulator design are not all encompassing and other methods are reported in the literature:

(1) CAVEAT: Bartlett *et al.*,1989, in "Chemical and Biological Problems in Molecular Recognition", Roberts, S.M.; Ley, S.V.; Campbell, M.M. eds.; Royal Society of Chemistry: Cambridge, pp182-196.

(2) FLOG: Miller et al., 1994, *J. Comp. Aided Molec. Design 8*:153.

(3) PRO Modulator: Clark *et al.*, 1995, *J. Comp. Aided Molec. Design 9*:13.

(4) MCSS: Miranker and Karplus, 1991, *Proteins: Structure, Function, and Genetics 11*:29.

(5) AUTODOCK: Goodsell and Olson, 1990, *Proteins: Structure, Function, and Genetics 8*:195.

(6) GRID: Goodford, 1985, *J. Med. Chem. 28*:849.

## Design by Modifying Compounds in Complex with PTKs

Another way of identifying compounds as potential modulators is to modify an existing modulator in the polypeptide active-site. For example, the computer representation of modulators can be modified within the computer representation of a PTK active-site. Detailed instructions for this technique can be found in the Molecular Simulations User Manual, 1995 in LUDI. The computer representation of the modulator is modified by the deletion of a chemical group or groups or by the addition of a chemical group or groups.

Upon each modification to the compound, the atoms of the modified compound and active-site can be shifted in conformation and the distance between the modulator and the active-site atoms may be scored along with any complimentary interactions formed between the two molecules. Scoring can be complete when a favorable geometric fit and favorable complementary interactions are attained. Compounds that have favorable scores are potential modulators of PTK function.

Design by Modifying the Structure of Compounds that Bind PTKs

A third method of structure-based modulator design is to screen compounds designed by a modulator building or modulator searching computer program. Examples of these types of programs can be found in the Molecular Simulations Package, Catalyst. Descriptions for using this program are documented in the Molecular Simulations User Guide (1995). Other computer programs used in this application are ISIS/HOST, ISIS/BASE, ISIS/DRAW) from Molecular Designs Limited and UNITY from Tripos Associates.

These programs can be operated on the structure of a compound that has been removed from the active-site of the three dimensional structure of a compound-PTK complex. Operating the program on such a compound is preferable since it is in a biologically active conformation.

A modulator construction computer program is a computer program that may be used to replace computer representations of chemical groups in a compound complexed with a PTK with groups from a computer data base. A modulator searching computer program is a computer program that may be used to search computer representations of compounds from a computer data base that have similar three dimensional structures and similar chemical groups as compound bound to a PTK.

A typical program can operate by using the following general steps:

(a) map the compounds by chemical features such as by hydrogen bond donors or acceptors, hydrophobic/lipophilic sites, positively ionizable sites, or negatively ionizable sites;

(b) add geometric constraints to the mapped features; and

(c) search data bases with the model generated in (b).

Those skilled in the art recognize that for indolinones, the important chemical features include, but are not limited to, a hydrogen bond donor, a hydrogen bond acceptor, and two hydrophobic points of contact. Those skilled in the art also recognize that not all of the possible chemical features of the compound need be present in the model of (b). One can use any subset of the model to generate different models for data base searches.

## IX. Organic Synthetic Techniques

The versatility of computer-based modulator design and identification lies in the diversity of structures screened by the computer programs. The computer programs can search data bases that contain 200,000 molecules and can modify modulators already complexed with the enzyme with a wide variety of chemical functional groups. A consequence of this chemical diversity is that a potential modulator of PTK function may take a chemical form that is not predictable. A wide array of organic synthetic techniques exist in the art to meet the challenge of constructing these potential modulators of PTK function. Many of these organic synthetic methods are described in detail in standard reference sources utilized by those skilled in the art. One example of such a reference is March, 1994, Advanced Organic Chemistry; Reactions, Mechanisms, and Structure, New York, McGraw Hill. Thus, the techniques required to synthesize a potential modulator of PTK function identified by computer-based methods are readily available to those skilled in the art of organic chemical synthesis.

## X. Cellular Assays Measuring the Effect of a PTK Modulator in Signal Transduction Pathways

Cellular assays can be used to test the activity of a potential modulator of PTK function as well as diagnose a disease associated with inappropriate PTK activity. A potential modulator of PTK function can be tested for activity *in vitro* by assays that measure the effect of a potential modulator on the autophosphorylation of a particular PTK over-expressed in a cell line. Thus, a modulator that acts as a potent inhibitor of the catalytic domain corresponding to a PTK would decrease the amount of autophosphorylation catalyzed by that PTK. Potential modulators could also be tested for activity in cell growth assays *in vitro* as well as in animal model assays *in vivo*.

*In vivo* assays are also useful for testing the bioactivity of a potential modulator designed by the methods of the invention.

Materials, methods, and experimental data for these assays are fully described in WO 96/40116 published on December 19, 1996, entitled "Indolinone Compounds for the Treatment of Disease". This application is incorporated herein by reference in its entirety, including all drawings, figures, and tables.

## XI. Administration of Modulators of PTK Function as Therapeutics for Disease

Methods of administering compounds to organisms as therapeutics for disease are fully described in WO 96/40116 published on December 19, 1996, entitled "Indolinone Compounds for the Treatment of Disease". This application is incorporated herein by reference in its entirety, including all drawings, figures, and tables.

## EXAMPLES

The examples below are non-limiting and are merely representative of various aspects and features of the present invention. The examples provide illustrative methods for obtaining crystalline forms of protein kinase polypeptides, methods for determining three dimensional structures of these protein kinase polypeptides, and methods for identifying modulators of protein kinases using the three dimensional structures of the protein kinases.

## EXAMPLE 1: X-ray Crystallographic Structure Determination of FGFR1

### Polypeptide Synthesis and Isolation

A recombinant baculovirus was engineered to encode residues 456-765 of human FGFR1. A cleavable N-terminal histidine tag was incorporated to aid in protein purification. Three amino acid substitutions were introduced: Cys-488 to Ala, Cys-584 to Ser and Leu-457 to Val. The two cysteine substitutions were made to prevent the formation of disulfide-linked oligomers, which occurs for the native protein. The substitution Leu-457 to Val introduced a *Ncol* cloning site near Met-456. The codon for Tyr-766 (TAC) was changed to a stop codon (TAG) and a *HindIII*-cloning site was generated following this stop codon. These substitutions were introduced into the full length human cDNA of FGFR1 in m13MPI9 by site-directed mutagenesis according to the manufacturer's protocol (Amersham).

The resulting construct was digested with *Ncol* and *HindIII* and was ligated into appropriately digested pBlueBac HistagB (Invitrogen). Transfection of insect cells (Sf9) was performed with the BaculoGold transfection system according to the manufacturer's protocol (Pharmingen). Following identification of positive plaques, the recombinant baculovirus was amplified to high titer ($5x10^7$ virus particles/ml). Sf9 cells were grown in 175-$cm^2$ flasks to a density of 2-$3x10^7$ per flask and infected with recombinant baculovirus with a multiplicity of infection (MOI) of 10.

After 48 hr, cells were harvested by centrifugation at 3,000g for 35 min at 4°C and then lysed in 25 mM HEPES (pH 7.5), 150 mM NaCl, 10% glycerol, 1.5 mM $MgCl_2$, 1 % Triton X-100, 10 μg/ml aprotonin, 10 μg/ml leupeptin, and 1 mM phenylmethylsulfonyl fluoride (PMSF). Lysates were centrifuged in a Sorval RC 5C (Dupont) for 1 hr at 4°C at 40,000g followed by ultracentrifugation in an XL-80 (Beckman) at 100,000g for 1 hr. After centrifugation, the clarified lysate was passed over a $Ni^{2+}$ -chelating column (Pharmacia), and the bound histidine-tagged fusion protein was eluted with 100 mM imidazole (pH 7.5). Pooled fractions were loaded onto a Mono Q anion exchange column (Pharmacia) and eluted with a NaCl gradient from 0 to 500 mM.

The fractions containing the fusion protein were concentrated in a Centricon-30 (Amicon), and the histidine tag was removed by overnight digestion with enterokinase (Biozyme) at 20°C. The digestion was terminated by the addition of aprotonin, leupeptin, PMSF, TPCK, and bovine pancreatic trypsin inhibitor (BPTI). The cleaved kinase domain was then separated from the histidine tag on a Superose 12 size-exclusion column (Pharmacia). The eluted kinase domain was further purified on a Mono Q column. The purified kinase domain was analyzed by N-terminal sequencing and mass spectrometry. Five amino acids (SAAGT) remained from the histidine tag. The predicted molecular mass was confirmed by mass spectrometry.

## Crystal Growth

Purified FGFR1 was concentrated to 20-50 mg/ml and exchanged into 10 mM Tris-HCl (pH 8.0), 10 mM NaCl, and

2 mM DTT using a Centricon-30. Crystals were grown at 4°C by vapor diffusion in hanging drops containing 2.0 $\mu$l of 10 mg/ml protein solution and 2.0 $\mu$l of reservoir solution: 16% polyethylene glycol (PEG) 10000, 0.3 M $(NH_4)_2SO_4$, 5% ethylene glycol, and 100 mM bis-Tris (pH 6.5).

Crystals of native FGFR1 were soaked in 500 ml stabilizing solution [25% PEG 10000, 0.3 M $(NH4)_2SO_4$, 0.1 M Bis-Tris (pH 6.5), 5% ethylene glycol] containing 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone (1-5 mM) or 3-[4-(4-formylpiperazine-1-yl)-benzylidenyl]-2-indolinone (1 mM) at 4°C for 24 to 48 hours. The final soaking concentration of DMSO was between 1 to 5%. The crystals cracked at higher concentrations of DMSO.

Co-crystals of FGFR1 with the inhibitors could also be obtained by vapor diffusion in hanging drops containing 2.0 $\mu$l of 10 mg/ml protein solution and 2.0 $\mu$l of reservoir solution containing 1 mM 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone and 3-[4-(4-formylpiperazine-1-yl-)benzylidenyl]-2-indolinone.

Co-crystals of FGFR1 complexed with AMP-PCP were obtained as described for the creation of native crystals, except that the protein solution additionally contained 10 mM AMP-PCP and 20 mM $MgCl_2$.

## Preparation Of Heavy Atom Derivative Crystals

Heavy atom derivative crystals were obtained by soaking FGFR1 native crystals (C2-A form) in a solution containing ethylmercurithiosalicylic acid (thimerosal),

$KAu(CN)_2$ or 4-chloromercuribenzoic acid, as provided in Table 1, *infra*,, and containing 25% PEG 10000, 0.3M $(NH_4)_2SO_4$,, 5% ethylene glycol or glycerol, and 100 mM bis-Tris (pH 6.5), and were flash-cooled either in liquid nitrogen directly (Synchrotron) or in a dry nitrogen stream at -175°C (rotating anode).

Data Collection and Structure Determination

For native crystals and crystals comprising the nucleotide analog AMP-PCP, data were collected either on a Rigaku RU-200 rotating anode operated at 50 kV and 100 mA (Cu Kα) and equipped with double-focusing mirrors and an R-AXIS IIC image plate detector, or at beamline X-4A at the National Synchrotron Light Source, Brookhaven National Laboratory. Synchrotron data (λ=1.07Å) were collected on Fuji image plates and read with a Fuji scanner. One cryo-cooled crystal was used for each of the data sets. To obtain cryo-cooled crystals, crystals were soaked in a cryo-protectant solution containing 25% PEG 10000, 0.3 M $(NH_4)_2SO_4$, 5% ethylene glycol or glycerol and 100 mM bis-Tris (pH 6.5), and were flash-cooled either in liquid nitrogen directly (synchrotron data) or in a dry nitrogen stream at -175°C (rotating anode data). All data were processed using DENZO and SCALEPACK. Otwinowski, 1993, "Oscillation data reduction program," Proceedings of the CCP4 Study Weekend, Sawyer et al., eds. (Daresbury, United Kingdom: SERC Daresbury Laboratory), 56-62.

For native crystals and crystals comprising the nucleotide analog AMP-PCP, a molecular replacement solution was found initially for the C2-B crystal form using an IRK search model that consisted of polyalanine with the common side chains for residues 993-1263 (FGFR1 residues 475-754), excluding residues 1094-1105 (kinase insert) and 1153-1170 (activation loop). With AMORE (Navaza, 1994, AmoRe: an automated package for molecular replacement," *Acta Crystallogr. A50*: 157-163), using 80% of the structure factor amplitudes between 15.0 and 3.5 Å, one of the two molecules in the asymmetric unit was located. The correlation coefficient (c.c.) for the correct 1-molecule solution was 0.23 (versus 0.20 for the highest incorrect solution). This molecule was rigid body-refined in X-PLOR (Brünger, 1992, X-PLOR (Version 3.1) Manual (New Haven, Conneticut: The Howeard Hughes Medical Institute and Department of Molecular Biophysics and Biochemistry, Yale Uiversity)), first as one rigid body unit, then as two units each comprising a lobe of the kinase. Rigid body refinement (12.0-3.5 Å, $F>3\sigma$) resulted in a relative rotation of the two lobes of ~10° and an increase of the c.c. from 0.20 to 0.25. The rigid body-refined molecule was then used as a new search model in AMORE, and this time both molecules in the asymmetric unit were located. The c.c. for the correct 2-molecule solution was 0.35 (versus 0.27 for the highest incorrect solution).

Multiple cycles of model building and refinement against 6.0-2.4 Å data resulted in the addition to the model of many of the side chains and some of the missing polypeptide chain. Model building was performed using TOM/FRODO (Jones, 1985, "Diffraction methods for biological macromolecules. Interactive computer graphics: FRODO," *Methods in Enzymology 115*: 157-171) and conjugate-gradient minimization and simulated annealing were performed using X-PLOR. Brünger, *supra*. At this stage, the R-value was 30% (free R-value of 36%). To help expedite model building and refinement, experimental phases were obtained. Because crystals grown in the presence of ethylene glycol were easier to manipulate than those grown in glycerol, several heavy-atom derivative data sets were collected from C2-A crystals that had been soaked in various heavy atom solutions. The C2-B structure was subsequently refined against 6.0-2.4 Å data to an R-value of 23.8% (free R-value of 30.4%) with r.m.s.d. values of 0.008 Å for bond distances and 1.4° for bond angles.

Molecular replacement was used to locate the two FGFR1 molecules (designated FLGK-A and FLGK-B) in the asymmetric unit of the C2-A crystal form. Using AMORE with 80% of structure factor amplitudes between 15.0 and 3.5 Å and the C2-B model, the c.c. for the correct 2-molecule solution was 0.62 (versus 0.35 for the highest incorrect solution). Heavy atom positions were determined from difference Fourier maps using the calculated phases from the partial model. Refinement of heavy atom parameters and phase determination were performed with MLPHARE (Otwinowski, 1991, "Maximum likelihood refinement of heavy atom parameters," *Isomorphous replacement and anomolous Ssattering*, Evans and Leslie eds. (Darsbury, United Kingdom: SERC Daresbury Laboratory), 56-62)). An initial molecular isomorphous replacement (MIR)-phased electron density map was calculated with data between 2.0. and 2.8 Å resolution. This map was improved by solvent flattening, histogram matching, and non-crystallographic symmetry (NCS) averaging using DM (Cowtan, 1994, "Protein Crystallography," *CCP4 and ESF-EACBM Newsletter (joint) 31*: 34-38).

Refinement of the C2-A FGFR1 structure against 6.0-2.0 Å data proceeded by conjugate-gradient minimization and simulated annealing using X-PLOR. Tight NCS restraints were imposed until data to 2.0 Å resolution were included in the refinement, at which point the restraints were lifted. An overall anisotropic B-value was calculated using X-PLOR and applied to the observed structure factors, reducing the R-value by ~3%. Water molecules whose B-values refined to ≥70 $Å^2$ were omitted from the subsequent refinement round. The average B-value is 37.5 $Å^2$ for all protein atoms, 35.4 $Å^2$ for protein atoms in FLGK-A, 39.7 $Å^2$ for protein atoms in FLGK-B, and 40.2 $Å^2$ for water molecules. The side chains for Cys-603 in FLGK-A and FLGK-B and for Met-534 in FLGK-B have been modeled in two different conformations. Residues that are not included in the atomic model due to poor supporting electron density are for FLGK-A: 456-463, 486-490, 501-504, 580-591, 763-765; and for FLG-B: 456-460, 501-504, 578-593, 646-651, 657-659, 762-765.

The positions of the two AMP-PCP molecules (one per FGFR1 molecule) were easily identified in $2F_{obs(co\text{-}complex)}-F_{calc(FGFR1)}$ difference Fourier maps. The AMP-PCP molecule bound to FLGK-B is less tightly bound and has been modeled with an occupancy of 0.5.

Table A summarizes the X-ray crystallography data sets of FGFR1 derivative crystals that were used to determine the structures of crystalline FGFR1 and crystalline FGFR1:AMP-PCP co-complex of the invention.

TABLE 5

Data Collection and MIR Phasing Summary

| | Native | AMP-PCP | Thi-1[a] | Thi-2[a] | PCMB[a] | $KAu(CN)_2$ |
|---|---|---|---|---|---|---|
| X-ray source | X-4A | RU-200 | RU-200 | RU-200 | RU-200 | RU-200 |
| Resolution limit (Å) | 2.0 | 2.3 | 2.6 | 2.8 | 2.8 | 2.8 |
| Number of sites | — | — | 4 | 7 | 2 | 2 |
| Conc. (mM)/time (h) | — | — | 0.1/24 | 0.1/48 | 0.2/2 | 5.0/72 |
| $R_{sym}$[b](%) | 4.8(19.7)[c] | 4.5(23.3)[c] | 5.5 | 9.8 | 6.8 | 6.8 |
| Total observations | 122569 | 91324 | 55456 | 59488 | 67988 | 45303 |
| Unique reflections | 50771 | 31997 | 42820[d] | 35538[d] | 18619 | 18202 |
| Completeness (%) | 97.3(96.3)[c] | 95.5(93.7)[c] | 95.0 | 96.7 | 98.0 | 97.7 |
| Signal (%I>3σ) | 80.7(50.3)[c] | 79.6(51.7)[c] | 69.8 | 66.8 | 84.7 | 77.6 |
| $R_{iso}$[e](%) | — | — | 17.1 | 31.2 | 15.4 | 15.2 |
| Phasing power[f] | — | — | 1.8 | 2.0 | 1.0 | 0.9 |
| $R_{cullis}$[g](%) | — | — | 0.55 | 0.50 | 0.81 | 0.84 |
| Overall FOM[h] | 0.60 | | | | | |

[a] Thi-1, Thi-2; ethylmercurithiosalicylic acid (thimerosal); PCMB: 4-chloromercuribenzoic acid.

[b] $R_{sym} = 100 \times \Sigma_h \Sigma_i |I_i(h) - \langle I(h) \rangle| / \Sigma_h \Sigma_i I_i(h)$

[c] Value in parentheses is for the highest resolution shell.

[d] I(+h) and I(-h) processed as independent reflections. Anomalous scattering contributions were included.

[e] $R_{iso} = 100 \times \Sigma_h \,||F_p(h) \pm F_p(h)| - |F_{PH}(h)|| / \Sigma_h |F_p(h)|$, where $F_p$ and $F_{PH}$ are the native and derivative structure factors, respectively.

[f] Phasing power: r.m.s. heavy atom structure factor / r.m.s. lack of closure (for acentric reflections from 20.0 to 2.8Å).

[g] $R_{cullis} = 100 \times \Sigma_h \,||F_{PH}(h)| - F_{H(calc)}(h)| / \Sigma_h |F_{PH}(h) \pm F_p(h)|$ (for centric reflections from 20.0 to 2.8Å).

[h] Figure of merit: $\int P(\phi)\exp(i\phi)d\phi / \int P(\phi)d(\phi)$, where P is the probability distribution of the phase angle $\phi$.

For crystals comprising FGFR1 and compounds 1 and 2, data were collected on a Rigaku RU-200 rotating anode (Cu Kα) operating at 50 kV and 100 mA and equipped with double-focusing mirrors and an R-AXIS IIC image plate detector. One cryo-cooled crystal was used for each of the data sets. Crystals were soaked in a cryo-protectant [25% PEG 10000, 0.3 M $(NH_4)_2SO_4$, 5% ethylene glycol, 100 mM bis-Tris (pH 6.5), and 1 mM: 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone (hereafter referred to as compound 1) or 3-[4-(4-formylpiperazine-1-yl-)benzylidenyl]-2-indolinone (hereafter referred to as compound 2) and flash-cooled in a dry nitrogen stream at -175°C. Data were processed using DENZO and SCALEPACK. Otwinowski, 1993, *Proceedings of the CCP4 Study Weekend* (Daresbury, United Kingdom: SERC Daresbury Laboratory) pp 56-62.

A summary of the data collection parameters are included in the following Table 6:

TABLE 6

| | Resolution limit (Å) | Observations (N) | Completeness (%) | Redundancy | $R_{sym}^a$ (%) | Signal (I> σI) |
|---|---|---|---|---|---|---|
| compound 1 | 2.5 | 93535 | 97.6 (96.1) | 2.7 | 6.8 (23.0) | 11.8 |
| compound 2 | 2.4 | 94093 | 99.1 (97.9) | 3.3 | 6.3 (32.2) | 11.4 |

compound 1 structure: 550 residues, 252 water molecules, 2 compound 1 molecules (4589 atoms)
compound 2 structure: 550 residues, 248 water molecules, 2 compound 2 molecules (4646 atoms)

## Structure Analyses

Atomic superpositions were performed with TOSS

(Hendrickson, 1979). Per residue solvent accessible surface calculations were done with X-PLOR. The surface area buried in a dimer interface was calculated with GRASP (Nicholls *et al.*, 1991) using a probe radius of 1.4 Å. The stereochemical quality of the atomic model was monitored using PROCHECK (Laskowski *et al.*, 1993, PROCHECK: a computer program to check the stereochemical quality of protein structures," *J. Appl. Cryst. 26*: 283-291). As defined in PROCHECK, 93% of the residues in the model have main-chain torsion angles in the most favored Ramachandran regions. There are no residues in disallowed regions, and three residues in generously allowed regions: Arg-622 in FLGK-A and FLGK-B and Arg-554 in FLGK-A. The overall G-factor score is 0.42.

Table 7 summarizes the X-ray crystallography refinement parameters of the structures of crystalline FGFR1 and crystalline FGFR1:AMP-PCP co-complex of the invention. Table 8 summarizes the X-ray crystallography refinement parameters for the FGFR1/compound complexes.

## TABLE 7

Refinement Parameters

FGFR1: 550 residues, 252 water molecules (4589 atoms)

FGFR1:AMP-PCP: 550 residues, 238 water molecules, 2 AMP-PCP molecules (4638 atoms)

| Model | d-spacings (Å) | Reflections (N) | R-value[a] (%) | R.m.s.d. | | |
|---|---|---|---|---|---|---|
| | | | | bonds (Å) | angles (°) | B-values[b] (Å$^2$) |
| FGFR1: | 6.0-2.0 | 42548 | 21.3 (26.2)[c] | 0.008 | 1.3 | 1.6 |
| FGFR1:AMP-PCP: | 6.0-2.3 | 26729 | 20.1 (27.5)[c] | 0.009 | 1.4 | 1.7 |

[a]R-value = $100 \times \Sigma_h \,||F_{obs}(h)| - |F_{calc}(h)|| / \Sigma_h |F_{obs}(h)|$ for reflections with $F_{obs} > 2\sigma$.

[b] For bonded protein atoms.

[c] Value in parentheses is the free R-value (Brünger, 1993) determined from 5% of the data.

## TABLE 8

| Model | d-spacings (Å) | Reflections | R-value[i] (N) | bonds (Å) | angles (°) | B-values[j] (Å$^2$) |
|---|---|---|---|---|---|---|
| compound 1 | 6.0–2.4 | 42548 | 19.7 (27.0)[k] | 0.008 | 1.3 | 1.6 |
| compound 2 | 6.0–2.5 | 26729 | 20.0 (28.0)[k] | 0.008 | 1.4 | 1.7 |

[a] $R_{sym} = 100 \times S_h S_i |I_i(\mathbf{h}) - \dot{I}(\mathbf{h})^{\dot{O}}| / S_h S_i I_i(\mathbf{h})$

[c] Value in parentheses is for the highest resolution shell.

[i] $R\text{-value} = 100 \times S_h ||F_o(\mathbf{h})| - |F_c(\mathbf{h})|| / S_h |F_o(\mathbf{h})|$, where $F_o$ and $F_c$ are the observed and calculated structure factors, respectively ($F_o > 2s$).

[j] For bonded protein atoms.

[k] Value in parentheses is the free R-value determined from 5% of the data.

Atomic Structural Coordinates

Tables 1 and 2 provide the atomic structural coordinates of unphosphorylated FGFR1 and unphosphorylated FGFR1:AMP-PCP co-complex, respectively. In the Tables, coordinates for both of the FGFR1 molecules of the dimer comprising the asymmetric unit are provided. The amino acid residue numbers coincide with those used in FIG. 3. In the first FGFR1 molecule of the dimer the residue number is preceded by a 1, i.e., residue number 464 of the first FGFR1 molecule of the dimer is denoted by "1464". Tables 3 and 4 provide the atomic structural coordinates of FGFR1 in complex with indolinone compounds found to inhibit FGFR1 function.

The following abbreviations are used in the Tables:

"Atom Type" refers to the element whose coordinates are provided. The first letter in the column defines the element.

"A.A." refers to amino acid.

"X, Y and Z" provide the Cartesian coordinates of the element.

"B" is a thermal factor that measures movement of the atom around its atomic center.

"OCC" refers to occupancy, and represents the percentage of time the atom type occupies the particular coordinate. OCC values range from 0 to 1, with 1 being 100%.

"PRT1" or "PRT2" relate to occupancy, with PRT1 designating the coordinates of the atom when in the first conformation and PRT2 designating the coordinates of the atom when in the second or alternate conformation.

Structural coordinates for FGFR1 may be modified by mathematical manipulation. Such manipulations include, but are not limited to, crystallographic permutations of the raw structure coordinates, fractionalization of the raw structure coordinates, integer additions or subtractions to sets of the raw structure coordinates, inversion of the raw structure coordinates and any combination of the above.

In addition, the structural coordinates can be slightly modified and still render nearly identical three dimensional structures. Therefore, a measure of a unique set of structural coordinates is the root-mean-square deviation of the resulting structure. Structural coordinates that render three dimensional structures that deviate from one another by a root-mean-square deviation of less than 1.5 Å may be viewed as identical.

## EXAMPLE 2: Computer-Based Design of Modulators of PTK Function

Potential modulators of PTK function were designed and identified by operating the program Catalyst on the structure of 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone. The chemical features constraining the search model include a hydrogen bond donor, a hydrogen bond acceptor, and two hydrophobic points of contact. Approximately 40 compounds were identified as potential modulators of PTK function using this method.

The compounds identified by the method as potential modulators of PTK function were commercially available. These compounds were then tested for their ability to inhibit the FLK PTK in an enzyme linked immunosorbant assay (ELISA). The method of performing this assay is taught in WO 96/40116, entitled "Indolinone Compounds for the Treatment of Disease," published on December 19, 1996, invented by Tang et al., incorporated by reference herein in its entirety, including all figures, drawings, and tables. Flk-1 specific antibodies can be prepared from the following protocol:

1. Prepare a Tresyl-Activated Agarose/Flk-1-D column by incubating 10 ml of Tresyl-Activated Agarose with 20 mg of purified GST-Flk-1-D fusion protein

in 100mM sodium bicarbonate (pH 9.6) buffer overnight at 4°C.

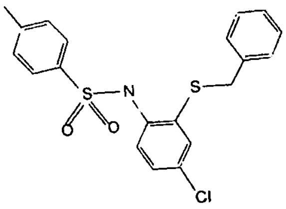
2. Wash the column once with PBS.
3. Block the excess sites on the column with 2 M glycine for 2 hours at 4°C.
4. Wash the column with PBS.
5. Incubate the column with Rabbit anti-Flk-1D production bleed for 2 hours at 4°C.
6. Wash the column with PBS.
7. Elute antiserum with 100 mM Citric Acid, pH3.0 and neutralize the eluate immediately with 2 M Tris, pH 9.0.
8. Dialyize the eluate against PBS overnight at 4oC with 3 changes of buffer (sample to buffer ratio is 1:100).
9. Adjust the dialyized antiserum to 5% glycerol and store at -80°C in small aliquotes.

The Flk-1 ELISA can include a 2,2-azino-bis(3-ethylbenz-thiazoline-6-sulfonic acid (ABTS) solution, which can comprise 100mM citric acid (anhydrous), 250 mM $Na_2HPO_4$ (pH 4.0), 0.5 mg/ml ABTS (Sigma catalog no. A-1888). The solution is most appropriately stored in dark at 4°C until ready for use.

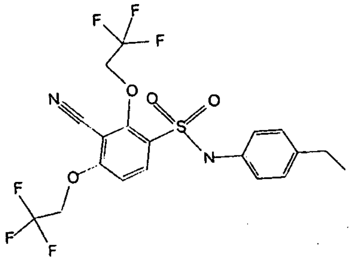
The FLK-1 specific antibodies can also be purchased from Santa Cruz Biotechnology (Catalog No. SC-504).

Four of the forty compounds identified as potential modulators of PTK function were potent modulators of FLK function. These molecules have the following structures:

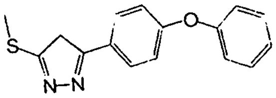
1



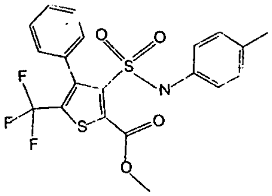
2



3



4



The modulators inhibit the FLK protein kinase with the following IC$_{50}$ values:

TABLE 9

| Compound | FLK kinase IC$_{50}$ ($\mu$M) compounds tested at 100$\mu$M | FLK kinase IC$_{50}$ ($\mu$M) compounds tested at 20$\mu$M | EGFR IC$_{50}$ ($\mu$M) | IGF-1R IC$_{50}$ ($\mu$M) |
|---|---|---|---|---|
| 1 | 14.8 | 14 | >100 | >100 |
| 2 | 15.7 | 10.6 | >100 | >100 |
| 3 | 21.4 | 16.6 | 68 | 30.9 |
| 4 | 22.9 | 16.4 | >100 | >100 |

The invention illustratively described herein may be practiced in the absence of any element or elements, limitation or limitations which is not specifically disclosed herein. The terms and expressions which have been employed are used as terms of description and not of limitation, and there is no intention that in the use of such terms and expressions of excluding any equivalents of the features shown and described or portions thereof, but it is recognized that various modifications are possible within the scope of the invention claimed. Thus, it should be understood that although the present invention has been specifically disclosed by preferred embodiments and optional features, modification and variation of the concepts herein disclosed may be resorted to by those skilled in the art, and that such modifications and variations are considered to be within the scope of this invention as defined by the appended claims.

Those references not previously incorporated herein by reference, including both patent and non-patent references, are expressly incorporated herein by reference for all purposes. Other embodiments are within the following claims.

## SEQUENCE LISTING

(1) GENERAL INFORMATION:

(i) APPLICANT: SUGEN, INCORPORATED
351 Galveston Drive
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(ii) TITLE OF INVENTION: CRYSTAL STRUCTURES OF A PROTEIN TYROSINE KINASE

(iii) NUMBER OF SEQUENCES: 5

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(B) STREET: 633 West Fifth Street
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(C) CITY: Los Angeles
(D) STATE: California
(E) COUNTRY: U.S.A.
(F) ZIP: 90071-2066

(v) COMPUTER READABLE FORM:

(A) MEDIUM TYPE: 3.5" Diskette, 1.44 Mb storage
(B) COMPUTER: IBM Compatible
(C) OPERATING SYSTEM: IBM P.C. DOS 5.0
(D) SOFTWARE: FastSEQ for Windows 2.0

(vi) CURRENT APPLICATION DATA:

(A) APPLICATION NUMBER: To Be Assigned
(B) FILING DATE: Herewith
(C) CLASSIFICATION:

(vii) PRIOR APPLICATION DATA:

(A) APPLICATION NUMBER:
(B) FILING DATE:

(viii) ATTORNEY/AGENT INFORMATION:

(A) NAME: Warburg, Richard J.
(B) REGISTRATION NUMBER: 32,327
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(C) TELEX: 67-3510

(2) INFORMATION FOR SEQ ID NO:1:

(i) SEQUENCE CHARACTERISTICS:

(A) LENGTH: 310 amino acids
(B) TYPE: amino acid
(C) STRANDEDNESS: single
(D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(iii) HYPOTHETICAL: NO

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:1:

Met Leu Ala Gly Val Ser Glu Tyr Glu Leu Pro Glu Asp Pro Arg Trp
1 5 10 15

Glu Leu Pro Arg Asp Arg Leu Val Leu Gly Lys Pro Leu Gly Glu Gly
20 25 30

Cys Phe Gly Gln Val Val Leu Ala Glu Ala Ile Gly Leu Asp Lys Asp
35 40 45

Lys Pro Asn Arg Val Thr Lys Val Ala Val Lys Met Leu Lys Ser Asp
50 55 60

Ala Thr Glu Lys Asp Leu Ser Asp Leu Ile Ser Glu Met Glu Met Met
65 70 75 80

Lys Met Ile Gly Lys His Lys Asn Ile Ile Asn Leu Leu Gly Ala Cys
85 90 95

Thr Gln Asp Gly Pro Leu Tyr Val Ile Val Glu Tyr Ala Ser Lys Gly
100 105 110

Asn Leu Arg Glu Tyr Leu Gln Ala Arg Arg Pro Pro Gly Leu Glu Tyr
115 120 125

Cys Tyr Asn Pro Ser His Asn Pro Glu Glu Gln Leu Ser Ser Lys Asp
130 135 140

```
Leu Val Ser Cys Ala Tyr Gln Val Ala Arg Gly Met Glu Tyr Leu Ala
145                 150                 155                 160

Ser Lys Lys Cys Ile His Arg Asp Leu Ala Ala Arg Asn Val Leu Val
                165                 170                 175

Thr Glu Asp Asn Val Met Lys Ile Ala Asp Phe Gly Leu Ala Arg Asp
            180                 185                 190

Ile His His Ile Asp Tyr Tyr Lys Lys Thr Thr Asn Gly Arg Leu Pro
        195                 200                 205

Val Lys Trp Met Ala Pro Glu Ala Leu Phe Asp Arg Ile Tyr Thr His
    210                 215                 220

Gln Ser Asp Val Trp Ser Phe Gly Val Leu Leu Trp Glu Ile Phe Thr
225                 230                 235                 240

Leu Gly Gly Ser Pro Tyr Pro Gly Val Pro Val Glu Glu Leu Phe Lys
                245                 250                 255

Leu Leu Lys Glu Gly His Arg Met Asp Lys Pro Ser Asn Cys Thr Asn
            260                 265                 270

Glu Leu Tyr Met Met Met Arg Asp Cys Trp His Ala Val Pro Ser Gln
        275                 280                 285

Arg Pro Thr Phe Lys Gln Leu Val Glu Asp Leu Asp Arg Ile Val Ala
    290                 295                 300

Leu Thr Ser Asn Gln Glu
305                 310
```

(2) INFORMATION FOR SEQ ID NO:2:

(i) SEQUENCE CHARACTERISTICS:

(A) LENGTH: 315 amino acids
(B) TYPE: amino acid
(C) STRANDEDNESS: single
(D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(iii) HYPOTHETICAL: NO

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:2:

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Ser Ala Ala Gly Thr Met Val Ala Gly Val Ser Glu Tyr Glu Leu Pro
1               5                   10                  15

Glu Asp Pro Arg Trp Glu Leu Pro Arg Asp Arg Leu Val Leu Gly Lys
            20                  25                  30
```

```
Pro Leu Gly Glu Gly Ala Phe Gly Gln Val Val Leu Ala Glu Ala Ile
        35                  40                  45

Gly Leu Asp Lys Asp Lys Pro Asn Arg Val Thr Lys Val Ala Val Lys
    50                  55                  60

Met Leu Lys Ser Asp Ala Thr Glu Lys Asp Leu Ser Asp Leu Ile Ser
65                  70                  75                  80

Glu Met Glu Met Met Lys Met Ile Gly Lys His Lys Asn Ile Ile Asn
                85                  90                  95

Leu Leu Gly Ala Cys Thr Gln Asp Gly Pro Leu Tyr Val Ile Val Glu
            100                 105                 110

Tyr Ala Ser Lys Gly Asn Leu Arg Glu Tyr Leu Gln Ala Arg Arg Pro
        115                 120                 125

Pro Gly Leu Glu Tyr Ser Tyr Asn Pro Ser His Asn Pro Glu Glu Gln
    130                 135                 140

Leu Ser Ser Lys Asp Leu Val Ser Cys Ala Tyr Gln Val Ala Arg Gly
145                 150                 155                 160

Met Glu Tyr Leu Ala Ser Lys Lys Cys Ile His Arg Asp Leu Ala Ala
                165                 170                 175

Arg Asn Val Leu Val Thr Glu Asp Asn Val Met Lys Ile Ala Asp Phe
            180                 185                 190

Gly Leu Ala Arg Asp Ile His His Ile Asp Tyr Tyr Lys Lys Thr Thr
        195                 200                 205

Asn Gly Arg Leu Pro Val Lys Trp Met Ala Pro Glu Ala Leu Phe Asp
    210                 215                 220

Arg Ile Tyr Thr His Gln Ser Asp Val Trp Ser Phe Gly Val Leu Leu
225                 230                 235                 240

Trp Glu Ile Phe Thr Leu Gly Gly Ser Pro Tyr Pro Gly Val Pro Val
                245                 250                 255

Glu Glu Leu Phe Lys Leu Leu Lys Glu Gly His Arg Met Asp Lys Pro
            260                 265                 270

Ser Asn Cys Thr Asn Glu Leu Tyr Met Met Met Arg Asp Cys Trp His
        275                 280                 285

Ala Val Pro Ser Gln Arg Pro Thr Phe Lys Gln Leu Val Glu Asp Leu
    290                 295                 300

Asp Arg Ile Val Ala Leu Thr Ser Asn Gln Glu
305                 310                 315
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(2) INFORMATION FOR SEQ ID NO:3:

(i) SEQUENCE CHARACTERISTICS:

(A) LENGTH: 351 amino acids
(B) TYPE: amino acid
(C) STRANDEDNESS: single
(D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(iii) HYPOTHETICAL: NO

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:3:

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Met Arg Gly Ser His His His His His His Gly Met Ala Ser Met Thr
1               5                   10                  15

Gly Gly Gln Gln Met Gly Arg Asp Leu Tyr Asp Asp Asp Asp Lys Asp
            20                  25                  30

Pro Ser Ser Arg Ser Ala Ala Gly Thr Met Val Ala Gly Val Ser Glu
        35                  40                  45

Tyr Glu Leu Pro Glu Asp Pro Arg Trp Glu Leu Pro Arg Asp Arg Leu
    50                  55                  60

Val Leu Gly Lys Pro Leu Gly Glu Gly Ala Phe Gly Gln Val Val Leu
65                  70                  75                  80

Ala Glu Ala Ile Gly Leu Asp Lys Asp Lys Pro Asn Arg Val Thr Lys
                85                  90                  95

Val Ala Val Lys Met Leu Lys Ser Asp Ala Thr Glu Lys Asp Leu Ser
            100                 105                 110

Asp Leu Ile Ser Glu Met Glu Met Met Lys Met Ile Gly Lys His Lys
        115                 120                 125

Asn Ile Ile Asn Leu Leu Gly Ala Cys Thr Gln Asp Gly Pro Leu Tyr
    130                 135                 140

Val Ile Val Glu Tyr Ala Ser Lys Gly Asn Leu Arg Glu Tyr Leu Gln
145                 150                 155                 160

Ala Arg Arg Pro Pro Gly Leu Glu Tyr Ser Tyr Asn Pro Ser His Asn
                165                 170                 175

Pro Glu Glu Gln Leu Ser Ser Lys Asp Leu Val Ser Cys Ala Tyr Gln
            180                 185                 190

Val Ala Arg Gly Met Glu Tyr Leu Ala Ser Lys Lys Cys Ile His Arg
        195                 200                 205
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Asp Leu Ala Ala Arg Asn Val Leu Val Thr Glu Asp Asn Val Met Lys
210 215 220

Ile Ala Asp Phe Gly Leu Ala Arg Asp Ile His His Ile Asp Tyr Tyr
225 230 235 240

Lys Lys Thr Thr Asn Gly Arg Leu Pro Val Lys Trp Met Ala Pro Glu
245 250 255

Ala Leu Phe Asp Arg Ile Tyr Thr His Gln Ser Asp Val Trp Ser Phe
260 265 270

Gly Val Leu Leu Trp Glu Ile Phe Thr Leu Gly Gly Ser Pro Tyr Pro
275 280 285

Gly Val Pro Val Glu Glu Leu Phe Lys Leu Leu Lys Glu Gly His Arg
290 295 300

Met Asp Lys Pro Ser Asn Cys Thr Asn Glu Leu Tyr Met Met Met Arg
305 310 315 320

Asp Cys Trp His Ala Val Pro Ser Gln Arg Pro Thr Phe Lys Gln Leu
325 330 335

Val Glu Asp Leu Asp Arg Ile Val Ala Leu Thr Ser Asn Gln Glu
340 345 350

(2) INFORMATION FOR SEQ ID NO:4:

(i) SEQUENCE CHARACTERISTICS:

(A) LENGTH: 933 base pairs
(B) TYPE: nucleic acid
(C) STRANDEDNESS: double
(D) TOPOLOGY: linear

(ii) MOLECULE TYPE: cDNA to mRNA

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:4:

ATGCTAGCAG GGGTCTCTGA GTATGAGCTT CCCGAAGACC CTCGCTGGGA GCTGCCTCGG 60
GACAGACTGG TCTTAGGCAA ACCCCTGGGA GAGGGCTGCT TTGGGCAGGT GGTGTTGGCA 120
GAGGCTATCG GGCTGGACAA GGACAAACCC AACCGTGTGA CCAAAGTGGC TGTGAAGATG 180
TTGAAGTCGG ACGCAACAGA GAAAGACTTG TCAGACCTGA TCTCAGAAAT GGAGATGATG 240
AAGATGATCG GGAAGCATAA GAATATCATC AACCTGCTGG GGGCCTGCAC GCAGGATGGT 300
CCCTTGTATG TCATCGTGGA GTATGCCTCC AAGGGCAACC TGCGGGAGTA CCTGCAGGCC 360
CGGAGGCCCC CAGGGCTGGA ATACTGCTAC AACCCCAGCC ACAACCCAGA GGAGCAGCTC 420

TCCTCCAAGG ACCTGGTGTC CTGCGCCTAC CAGGTGGCCC GAGGCATGGA GTATCTGGCC 480

TCCAAGAAGT GCATACACCG AGACCTGGCA GCCAGGAATG TCCTGGTGAC AGAGGACAAT 540

GTGATGAAGA TAGCAGACTT TGGCCTCGCA CGGGACATTC ACCACATCGA CTACTATAAA 600

AAGACAACCA ACGGCCGACT GCCTGTGAAG TGGATGGCAC CCGAGGCATT ATTTGACCGG 660

ATCTACACCC ACCAGAGTGA TGTGTGGTCT TTCGGGGTGC TCCTGTGGGA GATCTTCACT 720

CTGGGCGGCT CCCCATACCC CGGTGTGCCT GTGGAGGAAC TTTTCAAGCT GCTGAAGGAG 780

GGTCACCGCA TGGACAAGCC CAGTAACTGC ACCAACGAGC TGTACATGAT GATGCGGGAC 840

TGCTGGCATG CAGTGCCCTC ACAGAGACCC ACCTTCAAGC AGCTGGTGGA AGACCTGGAC 900

CGCATCGTGG CCTTGACCTC CAACCAGGAG TAG 933

(2) INFORMATION FOR SEQ ID NO:5:

(i) SEQUENCE CHARACTERISTICS:

(A) LENGTH: 1056 base pairs
(B) TYPE: nucleic acid
(C) STRANDEDNESS: double
(D) TOPOLOGY: linear

(ii) MOLECULE TYPE: cDNA

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:5:

ATGCGGGGTT CTCATCATCA TCATCATCAT GGTATGGCTA GCATGACTGG TGGACAGCAA 60

ATGGGTCGGG ATCTGTACGA CGATGACGAT AAGGATCCGA GCTCGAGATC TGCAGCTGGT 120

ACCATGGTAG CAGGGGTCTC TGAGTATGAG CTTCCCGAAG ACCCTCGCTG GGAGCTGCCT 180

CGGGACAGAC TGGTCTTAGG CAAACCCCTG GGAGAGGGCG CCTTTGGGCA GGTGGTGTTG 240

GCAGAGGCTA TCGGGCTGGA CAAGGACAAA CCCAACCGTG TGACCAAAGT GGCTGTGAAG 300

ATGTTGAAGT CGGACGCAAC AGAGAAAGAC TTGTCAGACC TGATCTCAGA AATGGAGATG 360

ATGAAGATGA TCGGGAAGCA TAAGAATATC ATCAACCTGC TGGGGGCCTG CACGCAGGAT 420

GGTCCCTTGT ATGTCATCGT GGAGTATGCC TCCAAGGGCA ACCTGCGGGA GTACCTGCAG 480

GCCCGGAGGC CCCCAGGGCT GGAATACTCC TACAACCCCA GCCACAACCC AGAGGAGCAG 540

CTCTCCTCCA AGGACCTGGT GTCCTGCGCC TACCAGGTGG CCCGAGGCAT GGAGTATCTG 600

GCCTCCAAGA AGTGCATACA CCGAGACCTG GCAGCCAGGA ATGTCCTGGT GACAGAGGAC 660

AATGTGATGA AGATAGCAGA CTTTGGCCTC GCACGGGACA TTCACCACAT CGACTACTAT 720
AAAAAGACAA CCAACGGCCG ACTGCCTGTG AAGTGGATGG CACCCGAGGC ATTATTTGAC 780
CGGATCTACA CCCACCAGAG TGATGTGTGG TCTTTCGGGG TGCTCCTGTG GGAGATCTTC 840
ACTCTGGGCG GCTCCCCATA CCCCGGTGTG CCTGTGGAGG AACTTTTCAA GCTGCTGAAG 900
GAGGGTCACC GCATGGACAA GCCCAGTAAC TGCACCAACG AGCTGTACAT GATGATGCGG 960
GACTGCTGGC ATGCAGTGCC CTCACAGAGA CCCACCTTCA AGCAGCTGGT GGAAGACCTG 1020
GACCGCATCG TGGCCTTGAC CTCCAACCAG GAGTAG 1056

TABLE 1

| | Atom No. | Atom Type | A.A | A.A No. | X | Y | Z | OCC | B |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1 | N | GLU | 1464 | -13.639 | 16.975 | 8.571 | 1.00 | 54.29 |
| ATOM | 3 | CA | GLU | 1464 | -12.479 | 17.105 | 7.695 | 1.00 | 52.62 |
| ATOM | 4 | CB | GLU | 1464 | -11.400 | 17.974 | 8.349 | 1.00 | 54.64 |
| ATOM | 5 | C | GLU | 1464 | -11.914 | 15.738 | 7.319 | 1.00 | 49.74 |
| ATOM | 6 | O | GLU | 1464 | -11.845 | 15.407 | 6.136 | 1.00 | 52.04 |
| ATOM | 7 | N | LEU | 1465 | -11.562 | 14.925 | 8.310 | 1.00 | 44.95 |
| ATOM | 9 | CA | LEU | 1465 | -11.018 | 13.599 | 8.037 | 1.00 | 41.04 |
| ATOM | 10 | CB | LEU | 1465 | -10.236 | 13.066 | 9.235 | 1.00 | 40.18 |
| ATOM | 11 | CG | LEU | 1465 | -8.719 | 13.196 | 9.130 | 1.00 | 43.70 |
| ATOM | 12 | CD1 | LEU | 1465 | -8.346 | 14.654 | 8.891 | 1.00 | 46.74 |
| ATOM | 13 | CD2 | LEU | 1465 | -8.061 | 12.671 | 10.395 | 1.00 | 40.72 |
| ATOM | 14 | C | LEU | 1465 | -12.092 | 12.594 | 7.656 | 1.00 | 39.18 |
| ATOM | 15 | O | LEU | 1465 | -13.187 | 12.590 | 8.219 | 1.00 | 38.05 |
| ATOM | 16 | N | PRO | 1466 | -11.802 | 11.748 | 6.657 | 1.00 | 37.20 |
| ATOM | 17 | CD | PRO | 1466 | -10.597 | 11.793 | 5.810 | 1.00 | 36.41 |
| ATOM | 18 | CA | PRO | 1466 | -12.741 | 10.727 | 6.189 | 1.00 | 36.13 |
| ATOM | 19 | CB | PRO | 1466 | -12.110 | 10.262 | 4.878 | 1.00 | 37.50 |
| ATOM | 20 | CG | PRO | 1466 | -10.629 | 10.459 | 5.135 | 1.00 | 36.20 |
| ATOM | 21 | C | PRO | 1466 | -12.846 | 9.595 | 7.201 | 1.00 | 35.61 |
| ATOM | 22 | O | PRO | 1466 | -11.847 | 9.174 | 7.788 | 1.00 | 35.18 |
| ATOM | 23 | N | GLU | 1467 | -14.060 | 9.121 | 7.429 | 1.00 | 35.38 |
| ATOM | 25 | CA | GLU | 1467 | -14.268 | 8.053 | 8.377 | 1.00 | 35.43 |
| ATOM | 26 | CB | GLU | 1467 | -15.744 | 7.965 | 8.746 | 1.00 | 41.10 |
| ATOM | 27 | CG | GLU | 1467 | -16.375 | 9.280 | 9.098 | 1.00 | 48.25 |
| ATOM | 28 | CD | GLU | 1467 | -17.819 | 9.145 | 9.596 | 1.00 | 50.24 |
| ATOM | 29 | OE1 | GLU | 1467 | -18.446 | 8.071 | 9.378 | 1.00 | 52.82 |
| ATOM | 30 | OE2 | GLU | 1467 | -18.314 | 10.109 | 10.230 | 1.00 | 51.26 |
| ATOM | 31 | C | GLU | 1467 | -13.838 | 6.714 | 7.801 | 1.00 | 32.65 |
| ATOM | 32 | O | GLU | 1467 | -13.899 | 6.511 | 6.591 | 1.00 | 35.06 |
| ATOM | 33 | N | ASP | 1468 | -13.299 | 5.854 | 8.659 | 1.00 | 30.46 |
| ATOM | 35 | CA | ASP | 1468 | -12.883 | 4.516 | 8.262 | 1.00 | 28.85 |
| ATOM | 36 | CB | ASP | 1468 | -11.384 | 4.424 | 7.975 | 1.00 | 29.34 |
| ATOM | 37 | CG | ASP | 1468 | -10.985 | 3.072 | 7.408 | 1.00 | 27.57 |
| ATOM | 38 | OD1 | ASP | 1468 | -11.833 | 2.159 | 7.359 | 1.00 | 27.78 |
| ATOM | 39 | OD2 | ASP | 1468 | -9.817 | 2.916 | 7.003 | 1.00 | 30.64 |
| ATOM | 40 | C | ASP | 1468 | -13.252 | 3.564 | 9.384 | 1.00 | 29.29 |
| ATOM | 41 | O | ASP | 1468 | -12.481 | 3.364 | 10.336 | 1.00 | 27.76 |
| ATOM | 42 | N | PRO | 1469 | -14.435 | 2.939 | 9.268 | 1.00 | 28.99 |
| ATOM | 43 | CD | PRO | 1469 | -15.354 | 3.091 | 8.120 | 1.00 | 28.09 |
| ATOM | 44 | CA | PRO | 1469 | -14.971 | 1.987 | 10.244 | 1.00 | 30.01 |
| ATOM | 45 | CB | PRO | 1469 | -16.244 | 1.473 | 9.553 | 1.00 | 33.33 |
| ATOM | 46 | CG | PRO | 1469 | -16.665 | 2.630 | 8.690 | 1.00 | 30.53 |
| ATOM | 47 | C | PRO | 1469 | -14.012 | 0.848 | 10.563 | 1.00 | 28.96 |
| ATOM | 48 | O | PRO | 1469 | -14.085 | 0.251 | 11.636 | 1.00 | 28.52 |
| ATOM | 49 | N | ARG | 1470 | -13.106 | 0.556 | 9.631 | 1.00 | 27.59 |
| ATOM | 51 | CA | ARG | 1470 | -12.139 | -0.520 | 9.810 | 1.00 | 27.37 |
| ATOM | 52 | CB | ARG | 1470 | -11.301 | -0.707 | 8.533 | 1.00 | 28.84 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 53 | CG | ARG | 1470 | -12.049 | -1.279 | 7.317 | 1.00 | 30.57 |
| ATOM | 54 | CD | ARG | 1470 | -11.137 | -1.352 | 6.068 | 1.00 | 26.71 |
| ATOM | 55 | NE | ARG | 1470 | -10.489 | -0.068 | 5.793 | 1.00 | 31.26 |
| ATOM | 57 | CZ | ARG | 1470 | -9.603 | 0.151 | 4.823 | 1.00 | 32.60 |
| ATOM | 58 | NH1 | ARG | 1470 | -9.241 | -0.828 | 3.999 | 1.00 | 33.19 |
| ATOM | 61 | NH2 | ARG | 1470 | -9.067 | 1.359 | 4.686 | 1.00 | 28.65 |
| ATOM | 64 | C | ARG | 1470 | -11.180 | -0.285 | 10.981 | 1.00 | 29.21 |
| ATOM | 65 | O | ARG | 1470 | -10.757 | -1.230 | 11.641 | 1.00 | 28.47 |
| ATOM | 66 | N | TRP | 1471 | -10.909 | 0.977 | 11.280 | 1.00 | 27.80 |
| ATOM | 68 | CA | TRP | 1471 | -9.940 | 1.314 | 12.306 | 1.00 | 28.62 |
| ATOM | 69 | CB | TRP | 1471 | -8.729 | 1.944 | 11.609 | 1.00 | 24.97 |
| ATOM | 70 | CG | TRP | 1471 | -8.044 | 0.976 | 10.728 | 1.00 | 24.86 |
| ATOM | 71 | CD2 | TRP | 1471 | -7.156 | -0.060 | 11.144 | 1.00 | 28.00 |
| ATOM | 72 | CE2 | TRP | 1471 | -6.782 | -0.776 | 9.989 | 1.00 | 29.23 |
| ATOM | 73 | CE3 | TRP | 1471 | -6.642 | -0.460 | 12.389 | 1.00 | 26.59 |
| ATOM | 74 | CD1 | TRP | 1471 | -8.166 | 0.860 | 9.374 | 1.00 | 27.23 |
| ATOM | 75 | NE1 | TRP | 1471 | -7.413 | -0.192 | 8.922 | 1.00 | 30.10 |
| ATOM | 77 | CZ2 | TRP | 1471 | -5.912 | -1.866 | 10.036 | 1.00 | 28.70 |
| ATOM | 78 | CZ3 | TRP | 1471 | -5.778 | -1.545 | 12.435 | 1.00 | 27.18 |
| ATOM | 79 | CH2 | TRP | 1471 | -5.424 | -2.237 | 11.266 | 1.00 | 27.23 |
| ATOM | 80 | C | TRP | 1471 | -10.371 | 2.223 | 13.440 | 1.00 | 28.42 |
| ATOM | 81 | O | TRP | 1471 | -9.664 | 2.321 | 14.442 | 1.00 | 26.48 |
| ATOM | 82 | N | GLU | 1472 | -11.521 | 2.874 | 13.293 | 1.00 | 28.62 |
| ATOM | 84 | CA | GLU | 1472 | -11.981 | 3.823 | 14.297 | 1.00 | 27.16 |
| ATOM | 85 | CB | GLU | 1472 | -13.245 | 4.534 | 13.799 | 1.00 | 28.89 |
| ATOM | 86 | CG | GLU | 1472 | -13.552 | 5.869 | 14.520 | 1.00 | 29.09 |
| ATOM | 87 | CD | GLU | 1472 | -12.692 | 7.042 | 14.054 | 1.00 | 26.43 |
| ATOM | 88 | OE1 | GLU | 1472 | -12.134 | 7.009 | 12.938 | 1.00 | 28.59 |
| ATOM | 89 | OE2 | GLU | 1472 | -12.596 | 8.024 | 14.801 | 1.00 | 27.28 |
| ATOM | 90 | C | GLU | 1472 | -12.217 | 3.269 | 15.701 | 1.00 | 25.10 |
| ATOM | 91 | O | GLU | 1472 | -12.763 | 2.196 | 15.861 | 1.00 | 26.48 |
| ATOM | 92 | N | LEU | 1473 | -11.750 | 3.991 | 16.711 | 1.00 | 24.65 |
| ATOM | 94 | CA | LEU | 1473 | -11.962 | 3.608 | 18.104 | 1.00 | 26.27 |
| ATOM | 95 | CB | LEU | 1473 | -10.645 | 3.266 | 18.817 | 1.00 | 28.24 |
| ATOM | 96 | CG | LEU | 1473 | -10.750 | 3.025 | 20.337 | 1.00 | 27.23 |
| ATOM | 97 | CD1 | LEU | 1473 | -11.323 | 1.636 | 20.642 | 1.00 | 25.23 |
| ATOM | 98 | CD2 | LEU | 1473 | -9.390 | 3.183 | 21.000 | 1.00 | 26.33 |
| ATOM | 99 | C | LEU | 1473 | -12.546 | 4.856 | 18.740 | 1.00 | 26.52 |
| ATOM | 100 | O | LEU | 1473 | -12.122 | 5.973 | 18.411 | 1.00 | 25.16 |
| ATOM | 101 | N | PRO | 1474 | -13.610 | 4.703 | 19.554 | 1.00 | 28.52 |
| ATOM | 102 | CD | PRO | 1474 | -14.435 | 3.500 | 19.770 | 1.00 | 29.65 |
| ATOM | 103 | CA | PRO | 1474 | -14.215 | 5.870 | 20.207 | 1.00 | 29.18 |
| ATOM | 104 | CB | PRO | 1474 | -15.368 | 5.251 | 21.003 | 1.00 | 28.58 |
| ATOM | 105 | CG | PRO | 1474 | -15.768 | 4.097 | 20.154 | 1.00 | 28.17 |
| ATOM | 106 | C | PRO | 1474 | -13.173 | 6.528 | 21.124 | 1.00 | 29.75 |
| ATOM | 107 | O | PRO | 1474 | -12.427 | 5.841 | 21.828 | 1.00 | 31.78 |
| ATOM | 108 | N | ARG | 1475 | -13.107 | 7.849 | 21.097 | 1.00 | 30.76 |
| ATOM | 110 | CA | ARG | 1475 | -12.149 | 8.588 | 21.900 | 1.00 | 32.26 |
| ATOM | 111 | CB | ARG | 1475 | -12.362 | 10.083 | 21.743 | 1.00 | 31.58 |
| ATOM | 112 | CG | ARG | 1475 | -12.178 | 10.536 | 20.342 | 1.00 | 37.54 |
| ATOM | 113 | CD | ARG | 1475 | -12.048 | 12.027 | 20.206 | 1.00 | 36.96 |
| ATOM | 114 | NE | ARG | 1475 | -11.733 | 12.317 | 18.813 | 1.00 | 40.07 |
| ATOM | 116 | CZ | ARG | 1475 | -10.503 | 12.501 | 18.352 | 1.00 | 37.59 |
| ATOM | 117 | NH1 | ARG | 1475 | -9.470 | 12.447 | 19.186 | 1.00 | 34.89 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 120 | NH2 | ARG | 1475 | -10.308 | 12.669 | 17.049 | 1.00 | 34.54 |
| ATOM | 123 | C | ARG | 1475 | -12.173 | 8.261 | 23.371 | 1.00 | 35.58 |
| ATOM | 124 | O | ARG | 1475 | -11.135 | 8.318 | 24.036 | 1.00 | 37.03 |
| ATOM | 125 | N | ASP | 1476 | -13.356 | 7.958 | 23.889 | 1.00 | 36.68 |
| ATOM | 127 | CA | ASP | 1476 | -13.498 | 7.647 | 25.307 | 1.00 | 37.07 |
| ATOM | 128 | CB | ASP | 1476 | -14.967 | 7.759 | 25.740 | 1.00 | 37.87 |
| ATOM | 129 | CG | ASP | 1476 | -15.851 | 6.704 | 25.115 | 1.00 | 38.93 |
| ATOM | 130 | OD1 | ASP | 1476 | -15.412 | 6.015 | 24.179 | 1.00 | 43.75 |
| ATOM | 131 | OD2 | ASP | 1476 | -17.003 | 6.558 | 25.563 | 1.00 | 45.77 |
| ATOM | 132 | C | ASP | 1476 | -12.922 | 6.292 | 25.701 | 1.00 | 35.86 |
| ATOM | 133 | O | ASP | 1476 | -12.923 | 5.928 | 26.878 | 1.00 | 37.98 |
| ATOM | 134 | N | ARG | 1477 | -12.478 | 5.527 | 24.711 | 1.00 | 33.37 |
| ATOM | 136 | CA | ARG | 1477 | -11.889 | 4.221 | 24.961 | 1.00 | 31.84 |
| ATOM | 137 | CB | ARG | 1477 | -12.214 | 3.262 | 23.809 | 1.00 | 31.84 |
| ATOM | 138 | CG | ARG | 1477 | -13.693 | 2.965 | 23.580 | 1.00 | 29.70 |
| ATOM | 139 | CD | ARG | 1477 | -14.366 | 2.365 | 24.809 | 1.00 | 33.88 |
| ATOM | 140 | NE | ARG | 1477 | -14.596 | 3.372 | 25.838 | 1.00 | 33.86 |
| ATOM | 142 | CZ | ARG | 1477 | -14.845 | 3.102 | 27.113 | 1.00 | 34.14 |
| ATOM | 143 | NH1 | ARG | 1477 | -14.906 | 1.846 | 27.542 | 1.00 | 30.58 |
| ATOM | 146 | NH2 | ARG | 1477 | -15.024 | 4.102 | 27.961 | 1.00 | 33.14 |
| ATOM | 149 | C | ARG | 1477 | -10.373 | 4.338 | 25.105 | 1.00 | 31.30 |
| ATOM | 150 | O | ARG | 1477 | -9.679 | 3.362 | 25.365 | 1.00 | 32.32 |
| ATOM | 151 | N | LEU | 1478 | -9.856 | 5.544 | 24.978 | 1.00 | 32.85 |
| ATOM | 153 | CA | LEU | 1478 | -8.426 | 5.739 | 25.054 | 1.00 | 35.64 |
| ATOM | 154 | CB | LEU | 1478 | -7.964 | 6.360 | 23.737 | 1.00 | 34.96 |
| ATOM | 155 | CG | LEU | 1478 | -6.498 | 6.291 | 23.331 | 1.00 | 36.36 |
| ATOM | 156 | CD1 | LEU | 1478 | -6.059 | 4.833 | 23.192 | 1.00 | 30.71 |
| ATOM | 157 | CD2 | LEU | 1478 | -6.335 | 7.048 | 22.020 | 1.00 | 33.97 |
| ATOM | 158 | C | LEU | 1478 | -8.054 | 6.625 | 26.243 | 1.00 | 37.60 |
| ATOM | 159 | O | LEU | 1478 | -8.366 | 7.815 | 26.263 | 1.00 | 41.20 |
| ATOM | 160 | N | VAL | 1479 | -7.442 | 6.023 | 27.257 | 1.00 | 36.52 |
| ATOM | 162 | CA | VAL | 1479 | -7.008 | 6.745 | 28.449 | 1.00 | 35.59 |
| ATOM | 163 | CB | VAL | 1479 | -7.041 | 5.829 | 29.688 | 1.00 | 35.92 |
| ATOM | 164 | CG1 | VAL | 1479 | -6.712 | 6.627 | 30.926 | 1.00 | 39.40 |
| ATOM | 165 | CG2 | VAL | 1479 | -8.404 | 5.163 | 29.825 | 1.00 | 34.46 |
| ATOM | 166 | C | VAL | 1479 | -5.577 | 7.224 | 28.197 | 1.00 | 35.36 |
| ATOM | 167 | O | VAL | 1479 | -4.622 | 6.443 | 28.269 | 1.00 | 32.50 |
| ATOM | 168 | N | LEU | 1480 | -5.439 | 8.506 | 27.878 | 1.00 | 37.77 |
| ATOM | 170 | CA | LEU | 1480 | -4.132 | 9.086 | 27.572 | 1.00 | 42.77 |
| ATOM | 171 | CB | LEU | 1480 | -4.298 | 10.421 | 26.842 | 1.00 | 41.84 |
| ATOM | 172 | CG | LEU | 1480 | -4.991 | 10.369 | 25.471 | 1.00 | 42.45 |
| ATOM | 173 | CD1 | LEU | 1480 | -5.135 | 11.774 | 24.924 | 1.00 | 42.58 |
| ATOM | 174 | CD2 | LEU | 1480 | -4.200 | 9.508 | 24.502 | 1.00 | 43.09 |
| ATOM | 175 | C | LEU | 1480 | -3.211 | 9.233 | 28.778 | 1.00 | 45.25 |
| ATOM | 176 | O | LEU | 1480 | -3.621 | 9.739 | 29.822 | 1.00 | 45.47 |
| ATOM | 177 | N | GLY | 1481 | -1.958 | 8.816 | 28.612 | 1.00 | 46.82 |
| ATOM | 179 | CA | GLY | 1481 | -1.016 | 8.889 | 29.708 | 1.00 | 50.47 |
| ATOM | 180 | C | GLY | 1481 | 0.296 | 9.617 | 29.472 | 1.00 | 52.24 |
| ATOM | 181 | O | GLY | 1481 | 0.360 | 10.638 | 28.781 | 1.00 | 53.41 |
| ATOM | 182 | N | LYS | 1482 | 1.349 | 9.070 | 30.068 | 1.00 | 53.64 |
| ATOM | 184 | CA | LYS | 1482 | 2.697 | 9.627 | 30.000 | 1.00 | 56.19 |
| ATOM | 185 | CB | LYS | 1482 | 3.636 | 8.776 | 30.859 | 1.00 | 57.19 |
| ATOM | 186 | CG | LYS | 1482 | 5.115 | 9.023 | 30.628 | 1.00 | 61.02 |
| ATOM | 187 | CD | LYS | 1482 | 5.938 | 7.831 | 31.089 | 1.00 | 63.12 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 188 | CE | LYS | 1482 | 5.494 | 6.547 | 30.395 | 1.00 | 61.98 |
| ATOM | 189 | NZ | LYS | 1482 | 6.252 | 5.368 | 30.899 | 1.00 | 63.38 |
| ATOM | 193 | C | LYS | 1482 | 3.297 | 9.795 | 28.604 | 1.00 | 56.56 |
| ATOM | 194 | O | LYS | 1482 | 3.291 | 8.868 | 27.791 | 1.00 | 55.03 |
| ATOM | 195 | N | PRO | 1483 | 3.852 | 10.983 | 28.323 | 1.00 | 58.31 |
| ATOM | 196 | CD | PRO | 1483 | 3.859 | 12.191 | 29.167 | 1.00 | 56.98 |
| ATOM | 197 | CA | PRO | 1483 | 4.465 | 11.254 | 27.020 | 1.00 | 59.52 |
| ATOM | 198 | CB | PRO | 1483 | 4.910 | 12.711 | 27.155 | 1.00 | 58.75 |
| ATOM | 199 | CG | PRO | 1483 | 3.927 | 13.278 | 28.141 | 1.00 | 58.79 |
| ATOM | 200 | C | PRO | 1483 | 5.673 | 10.335 | 26.834 | 1.00 | 61.17 |
| ATOM | 201 | O | PRO | 1483 | 6.509 | 10.216 | 27.731 | 1.00 | 61.31 |
| ATOM | 202 | N | LEU | 1484 | 5.728 | 9.643 | 25.702 | 1.00 | 64.31 |
| ATOM | 204 | CA | LEU | 1484 | 6.838 | 8.738 | 25.408 | 1.00 | 67.77 |
| ATOM | 205 | CB | LEU | 1484 | 6.349 | 7.512 | 24.640 | 1.00 | 67.66 |
| ATOM | 206 | CG | LEU | 1484 | 5.415 | 6.558 | 25.386 | 1.00 | 69.00 |
| ATOM | 207 | CD1 | LEU | 1484 | 4.943 | 5.457 | 24.445 | 1.00 | 66.76 |
| ATOM | 208 | CD2 | LEU | 1484 | 6.126 | 5.972 | 26.604 | 1.00 | 67.77 |
| ATOM | 209 | C | LEU | 1484 | 7.934 | 9.431 | 24.608 | 1.00 | 70.82 |
| ATOM | 210 | O | LEU | 1484 | 9.117 | 9.115 | 24.759 | 1.00 | 71.82 |
| ATOM | 211 | N | GLY | 1485 | 7.534 | 10.357 | 23.742 | 1.00 | 73.28 |
| ATOM | 213 | CA | GLY | 1485 | 8.492 | 11.077 | 22.922 | 1.00 | 74.53 |
| ATOM | 214 | C | GLY | 1485 | 7.819 | 11.754 | 21.747 | 1.00 | 75.19 |
| ATOM | 215 | O | GLY | 1485 | 6.635 | 12.090 | 21.822 | 1.00 | 75.61 |
| ATOM | 216 | N | GLN | 1491 | 4.406 | 14.274 | 18.638 | 1.00 | 50.72 |
| ATOM | 218 | CA | GLN | 1491 | 4.042 | 13.876 | 19.994 | 1.00 | 47.33 |
| ATOM | 219 | CB | GLN | 1491 | 3.033 | 14.869 | 20.587 | 1.00 | 46.67 |
| ATOM | 220 | C | GLN | 1491 | 3.486 | 12.449 | 20.073 | 1.00 | 46.66 |
| ATOM | 221 | O | GLN | 1491 | 2.581 | 12.074 | 19.323 | 1.00 | 45.20 |
| ATOM | 222 | N | VAL | 1492 | 4.072 | 11.650 | 20.960 | 1.00 | 45.41 |
| ATOM | 224 | CA | VAL | 1492 | 3.646 | 10.274 | 21.184 | 1.00 | 43.83 |
| ATOM | 225 | CB | VAL | 1492 | 4.680 | 9.244 | 20.709 | 1.00 | 41.60 |
| ATOM | 226 | CG1 | VAL | 1492 | 4.138 | 7.849 | 20.937 | 1.00 | 41.35 |
| ATOM | 227 | CG2 | VAL | 1492 | 5.007 | 9.445 | 19.237 | 1.00 | 42.72 |
| ATOM | 228 | C | VAL | 1492 | 3.458 | 10.084 | 22.683 | 1.00 | 44.45 |
| ATOM | 229 | O | VAL | 1492 | 4.335 | 10.437 | 23.482 | 1.00 | 43.86 |
| ATOM | 230 | N | VAL | 1493 | 2.309 | 9.548 | 23.070 | 1.00 | 42.67 |
| ATOM | 232 | CA | VAL | 1493 | 2.029 | 9.321 | 24.477 | 1.00 | 41.05 |
| ATOM | 233 | CB | VAL | 1493 | 0.884 | 10.242 | 25.013 | 1.00 | 40.64 |
| ATOM | 234 | CG1 | VAL | 1493 | 1.177 | 11.693 | 24.722 | 1.00 | 42.40 |
| ATOM | 235 | CG2 | VAL | 1493 | -0.459 | 9.844 | 24.427 | 1.00 | 43.36 |
| ATOM | 236 | C | VAL | 1493 | 1.626 | 7.880 | 24.704 | 1.00 | 40.09 |
| ATOM | 237 | O | VAL | 1493 | 1.129 | 7.212 | 23.796 | 1.00 | 39.99 |
| ATOM | 238 | N | LEU | 1494 | 1.927 | 7.374 | 25.890 | 1.00 | 37.10 |
| ATOM | 240 | CA | LEU | 1494 | 1.535 | 6.036 | 26.250 | 1.00 | 35.08 |
| ATOM | 241 | CB | LEU | 1494 | 2.359 | 5.542 | 27.440 | 1.00 | 35.57 |
| ATOM | 242 | CG | LEU | 1494 | 2.036 | 4.161 | 28.007 | 1.00 | 36.87 |
| ATOM | 243 | CD1 | LEU | 1494 | 2.123 | 3.085 | 26.931 | 1.00 | 36.90 |
| ATOM | 244 | CD2 | LEU | 1494 | 2.998 | 3.860 | 29.143 | 1.00 | 41.99 |
| ATOM | 245 | C | LEU | 1494 | 0.077 | 6.236 | 26.648 | 1.00 | 33.31 |
| ATOM | 246 | O | LEU | 1494 | -0.311 | 7.318 | 27.097 | 1.00 | 32.93 |
| ATOM | 247 | N | ALA | 1495 | -0.740 | 5.219 | 26.435 | 1.00 | 33.35 |
| ATOM | 249 | CA | ALA | 1495 | -2.147 | 5.292 | 26.773 | 1.00 | 30.67 |
| ATOM | 250 | CB | ALA | 1495 | -2.923 | 5.937 | 25.637 | 1.00 | 30.35 |
| ATOM | 251 | C | ALA | 1495 | -2.661 | 3.893 | 27.025 | 1.00 | 29.97 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 252 | O | ALA | 1495 | -1.944 | 2.909 | 26.840 | 1.00 | 28.15 |
| ATOM | 253 | N | GLU | 1496 | -3.898 | 3.813 | 27.488 | 1.00 | 30.37 |
| ATOM | 255 | CA | GLU | 1496 | -4.537 | 2.536 | 27.745 | 1.00 | 31.47 |
| ATOM | 256 | CB | GLU | 1496 | -4.862 | 2.392 | 29.223 | 1.00 | 32.48 |
| ATOM | 257 | CG | GLU | 1496 | -3.627 | 2.239 | 30.093 | 1.00 | 37.81 |
| ATOM | 258 | CD | GLU | 1496 | -3.938 | 2.426 | 31.565 | 1.00 | 41.09 |
| ATOM | 259 | OE1 | GLU | 1496 | -4.328 | 3.548 | 31.944 | 1.00 | 41.53 |
| ATOM | 260 | OE2 | GLU | 1496 | -3.797 | 1.453 | 32.341 | 1.00 | 44.12 |
| ATOM | 261 | C | GLU | 1496 | -5.806 | 2.524 | 26.916 | 1.00 | 32.72 |
| ATOM | 262 | O | GLU | 1496 | -6.586 | 3.478 | 26.954 | 1.00 | 33.91 |
| ATOM | 263 | N | ALA | 1497 | -5.953 | 1.494 | 26.094 | 1.00 | 31.06 |
| ATOM | 265 | CA | ALA | 1497 | -7.117 | 1.353 | 25.239 | 1.00 | 32.33 |
| ATOM | 266 | CB | ALA | 1497 | -6.691 | 0.879 | 23.859 | 1.00 | 29.56 |
| ATOM | 267 | C | ALA | 1497 | -8.056 | 0.343 | 25.885 | 1.00 | 32.26 |
| ATOM | 268 | O | ALA | 1497 | -7.648 | -0.773 | 26.197 | 1.00 | 33.55 |
| ATOM | 269 | N | ILE | 1498 | -9.286 | 0.759 | 26.160 | 1.00 | 32.99 |
| ATOM | 271 | CA | ILE | 1498 | -10.276 | -0.126 | 26.766 | 1.00 | 34.00 |
| ATOM | 272 | CB | ILE | 1498 | -11.329 | 0.668 | 27.592 | 1.00 | 34.69 |
| ATOM | 273 | CG2 | ILE | 1498 | -12.341 | -0.288 | 28.240 | 1.00 | 34.24 |
| ATOM | 274 | CG1 | ILE | 1498 | -10.647 | 1.496 | 28.686 | 1.00 | 33.56 |
| ATOM | 275 | CD1 | ILE | 1498 | -11.543 | 2.572 | 29.258 | 1.00 | 31.25 |
| ATOM | 276 | C | ILE | 1498 | -10.994 | -0.830 | 25.624 | 1.00 | 35.71 |
| ATOM | 277 | O | ILE | 1498 | -11.618 | -0.181 | 24.786 | 1.00 | 34.88 |
| ATOM | 278 | N | GLY | 1499 | -10.890 | -2.147 | 25.573 | 1.00 | 40.43 |
| ATOM | 280 | CA | GLY | 1499 | -11.553 | -2.884 | 24.516 | 1.00 | 47.63 |
| ATOM | 281 | C | GLY | 1499 | -10.670 | -3.233 | 23.330 | 1.00 | 53.08 |
| ATOM | 282 | O | GLY | 1499 | -9.934 | -4.226 | 23.380 | 1.00 | 54.97 |
| ATOM | 283 | N | LEU | 1500 | -10.713 | -2.394 | 22.294 | 1.00 | 54.18 |
| ATOM | 285 | CA | LEU | 1500 | -9.957 | -2.603 | 21.055 | 1.00 | 55.26 |
| ATOM | 286 | CB | LEU | 1500 | -8.444 | -2.726 | 21.305 | 1.00 | 55.39 |
| ATOM | 287 | CG | LEU | 1500 | -7.562 | -1.472 | 21.241 | 1.00 | 54.27 |
| ATOM | 288 | CD1 | LEU | 1500 | -6.110 | -1.891 | 21.367 | 1.00 | 52.89 |
| ATOM | 289 | CD2 | LEU | 1500 | -7.768 | -0.711 | 19.935 | 1.00 | 50.91 |
| ATOM | 290 | C | LEU | 1500 | -10.453 | -3.830 | 20.288 | 1.00 | 55.39 |
| ATOM | 291 | O | LEU | 1500 | -10.376 | -4.963 | 20.774 | 1.00 | 56.23 |
| ATOM | 292 | N | PRO | 1505 | -13.315 | -5.836 | 25.394 | 1.00 | 53.03 |
| ATOM | 293 | CD | PRO | 1505 | -13.945 | -7.148 | 25.167 | 1.00 | 55.12 |
| ATOM | 294 | CA | PRO | 1505 | -14.306 | -4.848 | 25.846 | 1.00 | 50.62 |
| ATOM | 295 | CB | PRO | 1505 | -15.635 | -5.607 | 25.715 | 1.00 | 50.09 |
| ATOM | 296 | CG | PRO | 1505 | -15.241 | -7.031 | 25.950 | 1.00 | 52.18 |
| ATOM | 297 | C | PRO | 1505 | -14.039 | -4.348 | 27.273 | 1.00 | 46.35 |
| ATOM | 298 | O | PRO | 1505 | -14.065 | -3.143 | 27.524 | 1.00 | 45.82 |
| ATOM | 299 | N | ASN | 1506 | -13.711 | -5.261 | 28.181 | 1.00 | 42.76 |
| ATOM | 301 | CA | ASN | 1506 | -13.433 | -4.892 | 29.566 | 1.00 | 45.29 |
| ATOM | 302 | CB | ASN | 1506 | -14.283 | -5.728 | 30.529 | 1.00 | 45.92 |
| ATOM | 303 | CG | ASN | 1506 | -15.752 | -5.395 | 30.441 | 1.00 | 46.17 |
| ATOM | 304 | OD1 | ASN | 1506 | -16.132 | -4.232 | 30.390 | 1.00 | 48.57 |
| ATOM | 305 | ND2 | ASN | 1506 | -16.589 | -6.418 | 30.406 | 1.00 | 48.63 |
| ATOM | 308 | C | ASN | 1506 | -11.954 | -5.008 | 29.939 | 1.00 | 45.33 |
| ATOM | 309 | O | ASN | 1506 | -11.597 | -5.084 | 31.121 | 1.00 | 44.53 |
| ATOM | 310 | N | ARG | 1507 | -11.100 | -5.010 | 28.924 | 1.00 | 45.63 |
| ATOM | 312 | CA | ARG | 1507 | -9.660 | -5.122 | 29.117 | 1.00 | 45.57 |
| ATOM | 313 | CB | ARG | 1507 | -9.131 | -6.354 | 28.375 | 1.00 | 53.33 |
| ATOM | 314 | CG | ARG | 1507 | -9.407 | -7.685 | 29.043 | 1.00 | 61.39 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 315 | CD | ARG | 1507 | -8.336 | -8.028 | 30.063 | 1.00 | 67.74 |
| ATOM | 316 | NE | ARG | 1507 | -8.525 | -9.376 | 30.585 | 1.00 | 74.64 |
| ATOM | 318 | CZ | ARG | 1507 | -7.970 | -9.842 | 31.701 | 1.00 | 80.01 |
| ATOM | 319 | NH1 | ARG | 1507 | -7.166 | -9.075 | 32.433 | 1.00 | 80.04 |
| ATOM | 322 | NH2 | ARG | 1507 | -8.268 | -11.068 | 32.115 | 1.00 | 83.41 |
| ATOM | 325 | C | ARG | 1507 | -8.964 | -3.897 | 28.555 | 1.00 | 40.94 |
| ATOM | 326 | O | ARG | 1507 | -9.370 | -3.375 | 27.517 | 1.00 | 37.60 |
| ATOM | 327 | N | VAL | 1508 | -7.956 | -3.409 | 29.267 | 1.00 | 39.33 |
| ATOM | 329 | CA | VAL | 1508 | -7.190 | -2.269 | 28.789 | 1.00 | 37.26 |
| ATOM | 330 | CB | VAL | 1508 | -6.854 | -1.224 | 29.905 | 1.00 | 36.25 |
| ATOM | 331 | CG1 | VAL | 1508 | -8.124 | -0.739 | 30.571 | 1.00 | 39.63 |
| ATOM | 332 | CG2 | VAL | 1508 | -5.903 | -1.796 | 30.928 | 1.00 | 36.92 |
| ATOM | 333 | C | VAL | 1508 | -5.898 | -2.818 | 28.188 | 1.00 | 34.38 |
| ATOM | 334 | O | VAL | 1508 | -5.387 | -3.851 | 28.630 | 1.00 | 32.85 |
| ATOM | 335 | N | THR | 1509 | -5.406 | -2.140 | 27.159 | 1.00 | 30.47 |
| ATOM | 337 | CA | THR | 1509 | -4.174 | -2.523 | 26.491 | 1.00 | 31.65 |
| ATOM | 338 | CB | THR | 1509 | -4.455 | -2.959 | 25.027 | 1.00 | 34.13 |
| ATOM | 339 | OG1 | THR | 1509 | -5.426 | -4.013 | 25.018 | 1.00 | 40.74 |
| ATOM | 341 | CG2 | THR | 1509 | -3.184 | -3.458 | 24.345 | 1.00 | 31.06 |
| ATOM | 342 | C | THR | 1509 | -3.270 | -1.299 | 26.461 | 1.00 | 28.38 |
| ATOM | 343 | O | THR | 1509 | -3.716 | -0.219 | 26.104 | 1.00 | 27.78 |
| ATOM | 344 | N | LYS | 1510 | -2.023 | -1.442 | 26.896 | 1.00 | 29.48 |
| ATOM | 346 | CA | LYS | 1510 | -1.101 | -0.312 | 26.835 | 1.00 | 30.54 |
| ATOM | 347 | CB | LYS | 1510 | 0.172 | -0.558 | 27.635 | 1.00 | 27.88 |
| ATOM | 348 | CG | LYS | 1510 | -0.037 | -0.600 | 29.118 | 1.00 | 33.91 |
| ATOM | 349 | CD | LYS | 1510 | 1.284 | -0.759 | 29.840 | 1.00 | 40.30 |
| ATOM | 350 | CE | LYS | 1510 | 1.145 | -1.674 | 31.062 | 1.00 | 46.24 |
| ATOM | 351 | NZ | LYS | 1510 | 0.338 | -1.096 | 32.187 | 1.00 | 49.09 |
| ATOM | 355 | C | LYS | 1510 | -0.757 | -0.166 | 25.365 | 1.00 | 28.64 |
| ATOM | 356 | O | LYS | 1510 | -0.402 | -1.142 | 24.704 | 1.00 | 28.76 |
| ATOM | 357 | N | VAL | 1511 | -0.902 | 1.048 | 24.856 | 1.00 | 29.34 |
| ATOM | 359 | CA | VAL | 1511 | -0.627 | 1.347 | 23.463 | 1.00 | 29.79 |
| ATOM | 360 | CB | VAL | 1511 | -1.951 | 1.457 | 22.658 | 1.00 | 27.14 |
| ATOM | 361 | CG1 | VAL | 1511 | -2.681 | 0.111 | 22.657 | 1.00 | 24.56 |
| ATOM | 362 | CG2 | VAL | 1511 | -2.837 | 2.561 | 23.243 | 1.00 | 22.15 |
| ATOM | 363 | C | VAL | 1511 | 0.123 | 2.672 | 23.361 | 1.00 | 29.83 |
| ATOM | 364 | O | VAL | 1511 | 0.213 | 3.413 | 24.338 | 1.00 | 33.14 |
| ATOM | 365 | N | ALA | 1512 | 0.705 | 2.939 | 22.196 | 1.00 | 27.86 |
| ATOM | 367 | CA | ALA | 1512 | 1.405 | 4.192 | 21.962 | 1.00 | 25.55 |
| ATOM | 368 | CB | ALA | 1512 | 2.743 | 3.935 | 21.297 | 1.00 | 24.69 |
| ATOM | 369 | C | ALA | 1512 | 0.500 | 5.009 | 21.057 | 1.00 | 25.25 |
| ATOM | 370 | O | ALA | 1512 | -0.061 | 4.483 | 20.107 | 1.00 | 27.18 |
| ATOM | 371 | N | VAL | 1513 | 0.340 | 6.289 | 21.360 | 1.00 | 29.63 |
| ATOM | 373 | CA | VAL | 1513 | -0.520 | 7.165 | 20.573 | 1.00 | 32.66 |
| ATOM | 374 | CB | VAL | 1513 | -1.704 | 7.713 | 21.422 | 1.00 | 32.47 |
| ATOM | 375 | CG1 | VAL | 1513 | -2.609 | 8.585 | 20.574 | 1.00 | 32.29 |
| ATOM | 376 | CG2 | VAL | 1513 | -2.508 | 6.559 | 22.031 | 1.00 | 32.15 |
| ATOM | 377 | C | VAL | 1513 | 0.238 | 8.334 | 19.938 | 1.00 | 34.67 |
| ATOM | 378 | O | VAL | 1513 | 0.792 | 9.185 | 20.635 | 1.00 | 34.65 |
| ATOM | 379 | N | LYS | 1514 | 0.207 | 8.367 | 18.605 | 1.00 | 36.88 |
| ATOM | 381 | CA | LYS | 1514 | 0.859 | 9.390 | 17.789 | 1.00 | 36.43 |
| ATOM | 382 | CB | LYS | 1514 | 1.349 | 8.764 | 16.489 | 1.00 | 36.37 |
| ATOM | 383 | CG | LYS | 1514 | 2.250 | 7.563 | 16.697 | 1.00 | 39.49 |
| ATOM | 384 | CD | LYS | 1514 | 2.559 | 6.854 | 15.390 | 1.00 | 45.29 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 385 | CE | LYS | 1514 | 3.080 | 7.815 | 14.331 | 1.00 | 50.70 |
| ATOM | 386 | NZ | LYS | 1514 | 4.212 | 8.685 | 14.798 | 1.00 | 51.41 |
| ATOM | 390 | C | LYS | 1514 | -0.121 | 10.496 | 17.459 | 1.00 | 36.75 |
| ATOM | 391 | O | LYS | 1514 | -1.228 | 10.234 | 16.978 | 1.00 | 35.42 |
| ATOM | 392 | N | MET | 1515 | 0.294 | 11.731 | 17.700 | 1.00 | 38.12 |
| ATOM | 394 | CA | MET | 1515 | -0.545 | 12.882 | 17.432 | 1.00 | 41.90 |
| ATOM | 395 | CB | MET | 1515 | -1.371 | 13.238 | 18.668 | 1.00 | 43.08 |
| ATOM | 396 | CG | MET | 1515 | -0.536 | 13.601 | 19.880 | 1.00 | 45.01 |
| ATOM | 397 | SD | MET | 1515 | -1.561 | 13.784 | 21.324 | 1.00 | 46.03 |
| ATOM | 398 | CE | MET | 1515 | -1.675 | 12.072 | 21.885 | 1.00 | 44.02 |
| ATOM | 399 | C | MET | 1515 | 0.314 | 14.065 | 17.021 | 1.00 | 44.65 |
| ATOM | 400 | O | MET | 1515 | 1.543 | 14.013 | 17.094 | 1.00 | 45.64 |
| ATOM | 401 | N | LEU | 1516 | -0.347 | 15.123 | 16.568 | 1.00 | 47.08 |
| ATOM | 403 | CA | LEU | 1516 | 0.329 | 16.337 | 16.134 | 1.00 | 48.08 |
| ATOM | 404 | CB | LEU | 1516 | -0.500 | 17.033 | 15.054 | 1.00 | 45.50 |
| ATOM | 405 | CG | LEU | 1516 | -0.764 | 16.265 | 13.764 | 1.00 | 43.22 |
| ATOM | 406 | CD1 | LEU | 1516 | -1.783 | 17.014 | 12.946 | 1.00 | 40.32 |
| ATOM | 407 | CD2 | LEU | 1516 | 0.540 | 16.072 | 12.991 | 1.00 | 43.78 |
| ATOM | 408 | C | LEU | 1516 | 0.516 | 17.302 | 17.297 | 1.00 | 51.27 |
| ATOM | 409 | O | LEU | 1516 | -0.214 | 17.249 | 18.291 | 1.00 | 50.37 |
| ATOM | 410 | N | LYS | 1517 | 1.491 | 18.191 | 17.157 | 1.00 | 55.47 |
| ATOM | 412 | CA | LYS | 1517 | 1.757 | 19.207 | 18.168 | 1.00 | 59.10 |
| ATOM | 413 | CB | LYS | 1517 | 3.203 | 19.702 | 18.068 | 1.00 | 61.61 |
| ATOM | 414 | CG | LYS | 1517 | 4.251 | 18.669 | 18.462 | 1.00 | 64.82 |
| ATOM | 415 | CD | LYS | 1517 | 5.635 | 19.109 | 18.018 | 1.00 | 67.42 |
| ATOM | 416 | CE | LYS | 1517 | 6.696 | 18.102 | 18.432 | 1.00 | 71.76 |
| ATOM | 417 | NZ | LYS | 1517 | 8.021 | 18.411 | 17.812 | 1.00 | 73.57 |
| ATOM | 421 | C | LYS | 1517 | 0.794 | 20.365 | 17.920 | 1.00 | 59.91 |
| ATOM | 422 | O | LYS | 1517 | 0.187 | 20.456 | 16.852 | 1.00 | 59.88 |
| ATOM | 423 | N | SER | 1518 | 0.686 | 21.267 | 18.886 | 1.00 | 61.85 |
| ATOM | 425 | CA | SER | 1518 | -0.216 | 22.409 | 18.760 | 1.00 | 63.70 |
| ATOM | 426 | CB | SER | 1518 | -0.158 | 23.274 | 20.024 | 1.00 | 64.21 |
| ATOM | 427 | C | SER | 1518 | 0.079 | 23.263 | 17.529 | 1.00 | 64.37 |
| ATOM | 428 | O | SER | 1518 | -0.841 | 23.757 | 16.875 | 1.00 | 66.16 |
| ATOM | 429 | N | ASP | 1519 | 1.359 | 23.410 | 17.202 | 1.00 | 64.15 |
| ATOM | 431 | CA | ASP | 1519 | 1.767 | 24.217 | 16.054 | 1.00 | 64.55 |
| ATOM | 432 | CB | ASP | 1519 | 3.109 | 24.897 | 16.343 | 1.00 | 65.84 |
| ATOM | 433 | C | ASP | 1519 | 1.858 | 23.441 | 14.742 | 1.00 | 63.95 |
| ATOM | 434 | O | ASP | 1519 | 2.432 | 23.931 | 13.769 | 1.00 | 64.95 |
| ATOM | 435 | N | ALA | 1520 | 1.303 | 22.232 | 14.719 | 1.00 | 62.57 |
| ATOM | 437 | CA | ALA | 1520 | 1.329 | 21.398 | 13.521 | 1.00 | 60.34 |
| ATOM | 438 | CB | ALA | 1520 | 0.704 | 20.039 | 13.810 | 1.00 | 60.53 |
| ATOM | 439 | C | ALA | 1520 | 0.616 | 22.062 | 12.353 | 1.00 | 58.21 |
| ATOM | 440 | O | ALA | 1520 | -0.464 | 22.631 | 12.506 | 1.00 | 58.32 |
| ATOM | 441 | N | THR | 1521 | 1.241 | 22.001 | 11.186 | 1.00 | 55.96 |
| ATOM | 443 | CA | THR | 1521 | 0.673 | 22.582 | 9.981 | 1.00 | 54.98 |
| ATOM | 444 | CB | THR | 1521 | 1.783 | 23.013 | 9.031 | 1.00 | 53.84 |
| ATOM | 445 | OG1 | THR | 1521 | 2.554 | 21.862 | 8.659 | 1.00 | 55.84 |
| ATOM | 447 | CG2 | THR | 1521 | 2.693 | 24.026 | 9.703 | 1.00 | 55.01 |
| ATOM | 448 | C | THR | 1521 | -0.184 | 21.545 | 9.261 | 1.00 | 54.25 |
| ATOM | 449 | O | THR | 1521 | -0.190 | 20.371 | 9.629 | 1.00 | 54.74 |
| ATOM | 450 | N | GLU | 1522 | -0.877 | 21.974 | 8.212 | 1.00 | 53.32 |
| ATOM | 452 | CA | GLU | 1522 | -1.702 | 21.066 | 7.423 | 1.00 | 52.64 |
| ATOM | 453 | CB | GLU | 1522 | -2.472 | 21.829 | 6.339 | 1.00 | 53.55 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 454 | C | GLU | 1522 | -0.793 | 20.012 | 6.780 | 1.00 | 51.95 |
| ATOM | 455 | O | GLU | 1522 | -1.226 | 18.895 | 6.504 | 1.00 | 53.28 |
| ATOM | 456 | N | LYS | 1523 | 0.464 | 20.377 | 6.544 | 1.00 | 48.66 |
| ATOM | 458 | CA | LYS | 1523 | 1.429 | 19.460 | 5.963 | 1.00 | 46.30 |
| ATOM | 459 | CB | LYS | 1523 | 2.730 | 20.201 | 5.620 | 1.00 | 48.30 |
| ATOM | 460 | CG | LYS | 1523 | 3.889 | 19.308 | 5.164 | 1.00 | 49.58 |
| ATOM | 461 | CD | LYS | 1523 | 3.487 | 18.388 | 4.016 | 1.00 | 50.87 |
| ATOM | 462 | CE | LYS | 1523 | 4.688 | 17.635 | 3.466 | 1.00 | 54.08 |
| ATOM | 463 | NZ | LYS | 1523 | 4.271 | 16.629 | 2.440 | 1.00 | 57.87 |
| ATOM | 467 | C | LYS | 1523 | 1.699 | 18.391 | 7.006 | 1.00 | 43.89 |
| ATOM | 468 | O | LYS | 1523 | 1.747 | 17.202 | 6.697 | 1.00 | 43.92 |
| ATOM | 469 | N | ASP | 1524 | 1.857 | 18.828 | 8.249 | 1.00 | 42.71 |
| ATOM | 471 | CA | ASP | 1524 | 2.114 | 17.915 | 9.351 | 1.00 | 42.11 |
| ATOM | 472 | CB | ASP | 1524 | 2.313 | 18.701 | 10.653 | 1.00 | 44.94 |
| ATOM | 473 | CG | ASP | 1524 | 3.623 | 19.490 | 10.673 | 1.00 | 48.90 |
| ATOM | 474 | OD1 | ASP | 1524 | 3.692 | 20.512 | 11.392 | 1.00 | 51.88 |
| ATOM | 475 | OD2 | ASP | 1524 | 4.590 | 19.084 | 9.990 | 1.00 | 50.06 |
| ATOM | 476 | C | ASP | 1524 | 0.956 | 16.931 | 9.481 | 1.00 | 39.85 |
| ATOM | 477 | O | ASP | 1524 | 1.164 | 15.738 | 9.748 | 1.00 | 39.01 |
| ATOM | 478 | N | LEU | 1525 | -0.261 | 17.438 | 9.296 | 1.00 | 38.32 |
| ATOM | 480 | CA | LEU | 1525 | -1.461 | 16.610 | 9.355 | 1.00 | 36.16 |
| ATOM | 481 | CB | LEU | 1525 | -2.720 | 17.470 | 9.200 | 1.00 | 35.13 |
| ATOM | 482 | CG | LEU | 1525 | -4.081 | 16.760 | 9.186 | 1.00 | 34.70 |
| ATOM | 483 | CD1 | LEU | 1525 | -4.184 | 15.668 | 10.252 | 1.00 | 36.15 |
| ATOM | 484 | CD2 | LEU | 1525 | -5.162 | 17.789 | 9.395 | 1.00 | 32.96 |
| ATOM | 485 | C | LEU | 1525 | -1.406 | 15.560 | 8.254 | 1.00 | 34.31 |
| ATOM | 486 | O | LEU | 1525 | -1.575 | 14.377 | 8.518 | 1.00 | 33.34 |
| ATOM | 487 | N | SER | 1526 | -1.136 | 16.005 | 7.030 | 1.00 | 36.40 |
| ATOM | 489 | CA | SER | 1526 | -1.039 | 15.128 | 5.865 | 1.00 | 37.16 |
| ATOM | 490 | CB | SER | 1526 | -0.669 | 15.931 | 4.618 | 1.00 | 38.84 |
| ATOM | 491 | OG | SER | 1526 | -1.736 | 16.779 | 4.245 | 1.00 | 49.61 |
| ATOM | 493 | C | SER | 1526 | -0.021 | 14.016 | 6.044 | 1.00 | 35.90 |
| ATOM | 494 | O | SER | 1526 | -0.273 | 12.873 | 5.670 | 1.00 | 36.68 |
| ATOM | 495 | N | ASP | 1527 | 1.142 | 14.349 | 6.591 | 1.00 | 35.89 |
| ATOM | 497 | CA | ASP | 1527 | 2.177 | 13.342 | 6.796 | 1.00 | 35.25 |
| ATOM | 498 | CB | ASP | 1527 | 3.497 | 13.998 | 7.201 | 1.00 | 35.58 |
| ATOM | 499 | CG | ASP | 1527 | 4.100 | 14.850 | 6.081 | 1.00 | 37.19 |
| ATOM | 500 | OD1 | ASP | 1527 | 3.750 | 14.653 | 4.895 | 1.00 | 37.38 |
| ATOM | 501 | OD2 | ASP | 1527 | 4.932 | 15.726 | 6.395 | 1.00 | 42.93 |
| ATOM | 502 | C | ASP | 1527 | 1.749 | 12.274 | 7.799 | 1.00 | 31.77 |
| ATOM | 503 | O | ASP | 1527 | 2.000 | 11.090 | 7.594 | 1.00 | 30.58 |
| ATOM | 504 | N | LEU | 1528 | 1.055 | 12.684 | 8.853 | 1.00 | 31.80 |
| ATOM | 506 | CA | LEU | 1528 | 0.581 | 11.730 | 9.857 | 1.00 | 33.53 |
| ATOM | 507 | CB | LEU | 1528 | -0.002 | 12.471 | 11.076 | 1.00 | 32.20 |
| ATOM | 508 | CG | LEU | 1528 | -0.440 | 11.623 | 12.275 | 1.00 | 32.63 |
| ATOM | 509 | CD1 | LEU | 1528 | 0.705 | 10.708 | 12.709 | 1.00 | 33.09 |
| ATOM | 510 | CD2 | LEU | 1528 | -0.891 | 12.512 | 13.426 | 1.00 | 31.52 |
| ATOM | 511 | C | LEU | 1528 | -0.468 | 10.792 | 9.235 | 1.00 | 32.89 |
| ATOM | 512 | O | LEU | 1528 | -0.494 | 9.589 | 9.521 | 1.00 | 32.39 |
| ATOM | 513 | N | ILE | 1529 | -1.336 | 11.357 | 8.393 | 1.00 | 33.72 |
| ATOM | 515 | CA | ILE | 1529 | -2.376 | 10.591 | 7.711 | 1.00 | 30.48 |
| ATOM | 516 | CB | ILE | 1529 | -3.336 | 11.505 | 6.895 | 1.00 | 28.85 |
| ATOM | 517 | CG2 | ILE | 1529 | -4.229 | 10.662 | 5.997 | 1.00 | 28.54 |
| ATOM | 518 | CG1 | ILE | 1529 | -4.200 | 12.344 | 7.843 | 1.00 | 29.52 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 519 | CD1 | ILE | 1529 | -5.143 | 13.308 | 7.133 | 1.00 | 32.07 |
| ATOM | 520 | C | ILE | 1529 | -1.698 | 9.608 | 6.768 | 1.00 | 31.50 |
| ATOM | 521 | O | ILE | 1529 | -2.009 | 8.419 | 6.780 | 1.00 | 30.75 |
| ATOM | 522 | N | SER | 1530 | -0.749 | 10.100 | 5.974 | 1.00 | 33.28 |
| ATOM | 524 | CA | SER | 1530 | -0.011 | 9.250 | 5.038 | 1.00 | 32.48 |
| ATOM | 525 | CB | SER | 1530 | 1.114 | 10.042 | 4.368 | 1.00 | 37.20 |
| ATOM | 526 | OG | SER | 1530 | 0.604 | 11.218 | 3.766 | 1.00 | 49.93 |
| ATOM | 528 | C | SER | 1530 | 0.583 | 8.045 | 5.756 | 1.00 | 29.05 |
| ATOM | 529 | O | SER | 1530 | 0.397 | 6.909 | 5.316 | 1.00 | 28.66 |
| ATOM | 530 | N | GLU | 1531 | 1.259 | 8.290 | 6.878 | 1.00 | 28.21 |
| ATOM | 532 | CA | GLU | 1531 | 1.880 | 7.207 | 7.631 | 1.00 | 27.30 |
| ATOM | 533 | CB | GLU | 1531 | 2.656 | 7.733 | 8.839 | 1.00 | 28.90 |
| ATOM | 534 | CG | GLU | 1531 | 3.271 | 6.609 | 9.672 | 1.00 | 27.17 |
| ATOM | 535 | CD | GLU | 1531 | 4.047 | 7.081 | 10.886 | 1.00 | 30.07 |
| ATOM | 536 | OE1 | GLU | 1531 | 4.779 | 6.244 | 11.448 | 1.00 | 34.78 |
| ATOM | 537 | OE2 | GLU | 1531 | 3.931 | 8.256 | 11.291 | 1.00 | 31.96 |
| ATOM | 538 | C | GLU | 1531 | 0.870 | 6.162 | 8.072 | 1.00 | 27.73 |
| ATOM | 539 | O | GLU | 1531 | 1.160 | 4.961 | 8.028 | 1.00 | 28.72 |
| ATOM | 540 | N | MET | 1532 | -0.286 | 6.621 | 8.555 | 1.00 | 29.78 |
| ATOM | 542 | CA | MET | 1532 | -1.373 | 5.734 | 8.990 | 1.00 | 28.79 |
| ATOM | 543 | CB | MET | 1532 | -2.501 | 6.553 | 9.646 | 1.00 | 28.90 |
| ATOM | 544 | CG | MET | 1532 | -3.763 | 5.741 | 9.993 | 1.00 | 29.73 |
| ATOM | 545 | SD | MET | 1532 | -5.089 | 6.693 | 10.765 | 1.00 | 30.19 |
| ATOM | 546 | CE | MET | 1532 | -5.455 | 7.870 | 9.494 | 1.00 | 26.70 |
| ATOM | 547 | C | MET | 1532 | -1.935 | 4.937 | 7.796 | 1.00 | 28.34 |
| ATOM | 548 | O | MET | 1532 | -2.166 | 3.730 | 7.893 | 1.00 | 26.62 |
| ATOM | 549 | N | GLU | 1533 | -2.165 | 5.624 | 6.678 | 1.00 | 28.85 |
| ATOM | 551 | CA | GLU | 1533 | -2.684 | 4.984 | 5.467 | 1.00 | 28.24 |
| ATOM | 552 | CB | GLU | 1533 | -2.936 | 6.027 | 4.384 | 1.00 | 25.42 |
| ATOM | 553 | CG | GLU | 1533 | -4.099 | 6.956 | 4.719 | 1.00 | 30.05 |
| ATOM | 554 | CD | GLU | 1533 | -5.393 | 6.201 | 5.021 | 1.00 | 29.47 |
| ATOM | 555 | OE1 | GLU | 1533 | -5.794 | 5.336 | 4.211 | 1.00 | 29.01 |
| ATOM | 556 | OE2 | GLU | 1533 | -6.011 | 6.472 | 6.073 | 1.00 | 33.98 |
| ATOM | 557 | C | GLU | 1533 | -1.694 | 3.944 | 4.968 | 1.00 | 28.01 |
| ATOM | 558 | O | GLU | 1533 | -2.072 | 2.845 | 4.573 | 1.00 | 27.39 |
| ATOM | 559 | N | MET | 1534 | -0.416 | 4.293 | 5.036 | 1.00 | 29.06 |
| ATOM | 561 | CA | MET | 1534 | 0.662 | 3.413 | 4.621 | 1.00 | 29.74 |
| ATOM | 562 | CB | MET | 1534 | 1.992 | 4.155 | 4.755 | 1.00 | 33.16 |
| ATOM | 563 | CG | MET | 1534 | 3.198 | 3.270 | 4.682 | 1.00 | 42.88 |
| ATOM | 564 | SD | MET | 1534 | 3.805 | 3.127 | 3.042 | 1.00 | 50.20 |
| ATOM | 565 | CE | MET | 1534 | 5.137 | 4.169 | 3.159 | 1.00 | 42.64 |
| ATOM | 566 | C | MET | 1534 | 0.641 | 2.156 | 5.493 | 1.00 | 26.90 |
| ATOM | 567 | O | MET | 1534 | 0.755 | 1.038 | 4.990 | 1.00 | 27.05 |
| ATOM | 568 | N | MET | 1535 | 0.512 | 2.348 | 6.803 | 1.00 | 25.42 |
| ATOM | 570 | CA | MET | 1535 | 0.437 | 1.233 | 7.737 | 1.00 | 25.88 |
| ATOM | 571 | CB | MET | 1535 | 0.325 | 1.741 | 9.181 | 1.00 | 27.63 |
| ATOM | 572 | CG | MET | 1535 | 1.607 | 2.391 | 9.737 | 1.00 | 27.26 |
| ATOM | 573 | SD | MET | 1535 | 1.584 | 2.561 | 11.564 | 1.00 | 29.49 |
| ATOM | 574 | CE | MET | 1535 | 1.294 | 4.255 | 11.699 | 1.00 | 28.22 |
| ATOM | 575 | C | MET | 1535 | -0.754 | 0.324 | 7.396 | 1.00 | 26.28 |
| ATOM | 576 | O | MET | 1535 | -0.645 | -0.908 | 7.469 | 1.00 | 25.93 |
| ATOM | 577 | N | LYS | 1536 | -1.890 | 0.928 | 7.032 | 1.00 | 27.19 |
| ATOM | 579 | CA | LYS | 1536 | -3.087 | 0.162 | 6.647 | 1.00 | 27.20 |
| ATOM | 580 | CB | LYS | 1536 | -4.257 | 1.088 | 6.310 | 1.00 | 25.29 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 581 | CG | LYS | 1536 | -4.897 | 1.770 | 7.491 | 1.00 | 23.86 |
| ATOM | 582 | CD | LYS | 1536 | -5.884 | 2.820 | 7.017 | 1.00 | 22.16 |
| ATOM | 583 | CE | LYS | 1536 | -6.460 | 3.588 | 8.174 | 1.00 | 22.25 |
| ATOM | 584 | NZ | LYS | 1536 | -7.484 | 4.541 | 7.713 | 1.00 | 23.40 |
| ATOM | 588 | C | LYS | 1536 | -2.785 | -0.699 | 5.423 | 1.00 | 24.52 |
| ATOM | 589 | O | LYS | 1536 | -3.069 | -1.889 | 5.403 | 1.00 | 26.61 |
| ATOM | 590 | N | MET | 1537 | -2.183 | -0.093 | 4.411 | 1.00 | 27.12 |
| ATOM | 592 | CA | MET | 1537 | -1.843 | -0.815 | 3.194 | 1.00 | 28.06 |
| ATOM | 593 | CB | MET | 1537 | -1.269 | 0.147 | 2.147 | 1.00 | 30.36 |
| ATOM | 594 | CG | MET | 1537 | -2.265 | 1.164 | 1.591 | 1.00 | 36.31 |
| ATOM | 595 | SD | MET | 1537 | -3.699 | 0.444 | 0.727 | 1.00 | 42.19 |
| ATOM | 596 | CE | MET | 1537 | -2.912 | -0.057 | -0.793 | 1.00 | 36.22 |
| ATOM | 597 | C | MET | 1537 | -0.857 | -1.952 | 3.447 | 1.00 | 26.98 |
| ATOM | 598 | O | MET | 1537 | -1.060 | -3.065 | 2.963 | 1.00 | 25.34 |
| ATOM | 599 | N | ILE | 1538 | 0.188 | -1.678 | 4.229 | 1.00 | 27.69 |
| ATOM | 601 | CA | ILE | 1538 | 1.234 | -2.674 | 4.535 | 1.00 | 25.39 |
| ATOM | 602 | CB | ILE | 1538 | 2.454 | -2.006 | 5.255 | 1.00 | 24.42 |
| ATOM | 603 | CG2 | ILE | 1538 | 3.424 | -3.051 | 5.811 | 1.00 | 25.28 |
| ATOM | 604 | CG1 | ILE | 1538 | 3.223 | -1.131 | 4.269 | 1.00 | 23.88 |
| ATOM | 605 | CD1 | ILE | 1538 | 4.373 | -0.372 | 4.901 | 1.00 | 27.19 |
| ATOM | 606 | C | ILE | 1538 | 0.760 | -3.922 | 5.292 | 1.00 | 25.59 |
| ATOM | 607 | O | ILE | 1538 | 1.242 | -5.033 | 5.035 | 1.00 | 26.11 |
| ATOM | 608 | N | GLY | 1539 | -0.193 | -3.767 | 6.208 | 1.00 | 26.13 |
| ATOM | 610 | CA | GLY | 1539 | -0.661 | -4.940 | 6.934 | 1.00 | 25.25 |
| ATOM | 611 | C | GLY | 1539 | 0.191 | -5.280 | 8.149 | 1.00 | 26.77 |
| ATOM | 612 | O | GLY | 1539 | 1.214 | -4.637 | 8.414 | 1.00 | 25.42 |
| ATOM | 613 | N | LYS | 1540 | -0.204 | -6.327 | 8.862 | 1.00 | 25.62 |
| ATOM | 615 | CA | LYS | 1540 | 0.467 | -6.716 | 10.092 | 1.00 | 26.38 |
| ATOM | 616 | CB | LYS | 1540 | -0.552 | -7.283 | 11.084 | 1.00 | 27.15 |
| ATOM | 617 | CG | LYS | 1540 | -1.573 | -6.303 | 11.550 | 1.00 | 34.23 |
| ATOM | 618 | CD | LYS | 1540 | -2.528 | -6.943 | 12.546 | 1.00 | 40.69 |
| ATOM | 619 | CE | LYS | 1540 | -3.559 | -5.927 | 13.057 | 1.00 | 44.08 |
| ATOM | 620 | NZ | LYS | 1540 | -2.956 | -4.800 | 13.833 | 1.00 | 44.05 |
| ATOM | 624 | C | LYS | 1540 | 1.609 | -7.705 | 10.014 | 1.00 | 24.37 |
| ATOM | 625 | O | LYS | 1540 | 1.627 | -8.600 | 9.181 | 1.00 | 26.12 |
| ATOM | 626 | N | HIS | 1541 | 2.545 | -7.538 | 10.936 | 1.00 | 24.41 |
| ATOM | 628 | CA | HIS | 1541 | 3.666 | -8.440 | 11.091 | 1.00 | 25.41 |
| ATOM | 629 | CB | HIS | 1541 | 4.772 | -8.228 | 10.057 | 1.00 | 21.88 |
| ATOM | 630 | CG | HIS | 1541 | 5.798 | -9.320 | 10.068 | 1.00 | 22.68 |
| ATOM | 631 | CD2 | HIS | 1541 | 5.823 | -10.522 | 9.444 | 1.00 | 21.40 |
| ATOM | 632 | ND1 | HIS | 1541 | 6.939 | -9.268 | 10.843 | 1.00 | 22.12 |
| ATOM | 634 | CE1 | HIS | 1541 | 7.619 | -10.389 | 10.697 | 1.00 | 24.78 |
| ATOM | 635 | NE2 | HIS | 1541 | 6.966 | -11.167 | 9.854 | 1.00 | 27.00 |
| ATOM | 637 | C | HIS | 1541 | 4.234 | -8.328 | 12.494 | 1.00 | 25.47 |
| ATOM | 638 | O | HIS | 1541 | 4.364 | -7.239 | 13.050 | 1.00 | 26.77 |
| ATOM | 639 | N | LYS | 1542 | 4.560 | -9.476 | 13.063 | 1.00 | 26.38 |
| ATOM | 641 | CA | LYS | 1542 | 5.127 | -9.552 | 14.401 | 1.00 | 30.07 |
| ATOM | 642 | CB | LYS | 1542 | 5.515 | -11.003 | 14.692 | 1.00 | 31.38 |
| ATOM | 643 | CG | LYS | 1542 | 6.061 | -11.252 | 16.077 | 1.00 | 42.79 |
| ATOM | 644 | CD | LYS | 1542 | 6.289 | -12.735 | 16.294 | 1.00 | 50.84 |
| ATOM | 645 | CE | LYS | 1542 | 7.041 | -13.374 | 15.114 | 1.00 | 56.75 |
| ATOM | 646 | NZ | LYS | 1542 | 7.511 | -14.763 | 15.424 | 1.00 | 61.29 |
| ATOM | 650 | C | LYS | 1542 | 6.342 | -8.652 | 14.624 | 1.00 | 27.65 |
| ATOM | 651 | O | LYS | 1542 | 6.519 | -8.113 | 15.711 | 1.00 | 26.83 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 652 | N | ASN | 1543 | 7.146 | -8.445 | 13.585 | 1.00 | 27.20 |
| ATOM | 654 | CA | ASN | 1543 | 8.354 | -7.642 | 13.735 | 1.00 | 25.50 |
| ATOM | 655 | CB | ASN | 1543 | 9.578 | -8.431 | 13.260 | 1.00 | 25.59 |
| ATOM | 656 | CG | ASN | 1543 | 9.712 | -9.767 | 13.974 | 1.00 | 22.64 |
| ATOM | 657 | OD1 | ASN | 1543 | 9.522 | -10.821 | 13.371 | 1.00 | 26.76 |
| ATOM | 658 | ND2 | ASN | 1543 | 9.970 | -9.727 | 15.273 | 1.00 | 25.56 |
| ATOM | 661 | C | ASN | 1543 | 8.374 | -6.213 | 13.226 | 1.00 | 25.48 |
| ATOM | 662 | O | ASN | 1543 | 9.417 | -5.692 | 12.842 | 1.00 | 24.58 |
| ATOM | 663 | N | ILE | 1544 | 7.209 | -5.575 | 13.244 | 1.00 | 24.60 |
| ATOM | 665 | CA | ILE | 1544 | 7.065 | -4.177 | 12.868 | 1.00 | 22.32 |
| ATOM | 666 | CB | ILE | 1544 | 6.524 | -3.972 | 11.409 | 1.00 | 25.82 |
| ATOM | 667 | CG2 | ILE | 1544 | 7.401 | -4.720 | 10.403 | 1.00 | 24.24 |
| ATOM | 668 | CG1 | ILE | 1544 | 5.057 | -4.411 | 11.279 | 1.00 | 26.04 |
| ATOM | 669 | CD1 | ILE | 1544 | 4.446 | -4.121 | 9.901 | 1.00 | 23.20 |
| ATOM | 670 | C | ILE | 1544 | 6.075 | -3.598 | 13.881 | 1.00 | 22.37 |
| ATOM | 671 | O | ILE | 1544 | 5.364 | -4.345 | 14.559 | 1.00 | 21.68 |
| ATOM | 672 | N | ILE | 1545 | 6.111 | -2.290 | 14.076 | 1.00 | 23.72 |
| ATOM | 674 | CA | ILE | 1545 | 5.169 | -1.650 | 14.989 | 1.00 | 25.92 |
| ATOM | 675 | CB | ILE | 1545 | 5.602 | -0.199 | 15.364 | 1.00 | 27.24 |
| ATOM | 676 | CG2 | ILE | 1545 | 4.452 | 0.554 | 16.035 | 1.00 | 22.76 |
| ATOM | 677 | CG1 | ILE | 1545 | 6.839 | -0.219 | 16.285 | 1.00 | 25.57 |
| ATOM | 678 | CD1 | ILE | 1545 | 6.591 | -0.797 | 17.686 | 1.00 | 24.66 |
| ATOM | 679 | C | ILE | 1545 | 3.877 | -1.612 | 14.179 | 1.00 | 26.03 |
| ATOM | 680 | O | ILE | 1545 | 3.823 | -0.988 | 13.122 | 1.00 | 25.70 |
| ATOM | 681 | N | ASN | 1546 | 2.849 | -2.293 | 14.669 | 1.00 | 24.79 |
| ATOM | 683 | CA | ASN | 1546 | 1.577 | -2.354 | 13.956 | 1.00 | 25.51 |
| ATOM | 684 | CB | ASN | 1546 | 0.922 | -3.727 | 14.137 | 1.00 | 25.17 |
| ATOM | 685 | CG | ASN | 1546 | 1.730 | -4.839 | 13.539 | 1.00 | 21.67 |
| ATOM | 686 | OD1 | ASN | 1546 | 1.856 | -4.947 | 12.329 | 1.00 | 24.29 |
| ATOM | 687 | ND2 | ASN | 1546 | 2.278 | -5.686 | 14.384 | 1.00 | 22.24 |
| ATOM | 690 | C | ASN | 1546 | 0.578 | -1.276 | 14.349 | 1.00 | 26.85 |
| ATOM | 691 | O | ASN | 1546 | 0.630 | -0.724 | 15.453 | 1.00 | 28.67 |
| ATOM | 692 | N | LEU | 1547 | -0.301 | -0.956 | 13.407 | 1.00 | 27.70 |
| ATOM | 694 | CA | LEU | 1547 | -1.357 | 0.019 | 13.622 | 1.00 | 27.64 |
| ATOM | 695 | CB | LEU | 1547 | -1.945 | 0.481 | 12.284 | 1.00 | 24.87 |
| ATOM | 696 | CG | LEU | 1547 | -3.173 | 1.400 | 12.337 | 1.00 | 23.25 |
| ATOM | 697 | CD1 | LEU | 1547 | -2.790 | 2.763 | 12.929 | 1.00 | 23.76 |
| ATOM | 698 | CD2 | LEU | 1547 | -3.757 | 1.569 | 10.923 | 1.00 | 23.47 |
| ATOM | 699 | C | LEU | 1547 | -2.415 | -0.771 | 14.396 | 1.00 | 27.27 |
| ATOM | 700 | O | LEU | 1547 | -2.663 | -1.952 | 14.103 | 1.00 | 25.27 |
| ATOM | 701 | N | LEU | 1548 | -3.000 | -0.130 | 15.400 | 1.00 | 27.94 |
| ATOM | 703 | CA | LEU | 1548 | -4.017 | -0.770 | 16.223 | 1.00 | 26.98 |
| ATOM | 704 | CB | LEU | 1548 | -3.623 | -0.735 | 17.708 | 1.00 | 24.65 |
| ATOM | 705 | CG | LEU | 1548 | -2.327 | -1.450 | 18.108 | 1.00 | 25.38 |
| ATOM | 706 | CD1 | LEU | 1548 | -2.189 | -1.428 | 19.613 | 1.00 | 25.73 |
| ATOM | 707 | CD2 | LEU | 1548 | -2.337 | -2.886 | 17.621 | 1.00 | 23.92 |
| ATOM | 708 | C | LEU | 1548 | -5.369 | -0.113 | 16.042 | 1.00 | 26.65 |
| ATOM | 709 | O | LEU | 1548 | -6.392 | -0.752 | 16.238 | 1.00 | 27.11 |
| ATOM | 710 | N | GLY | 1549 | -5.378 | 1.163 | 15.684 | 1.00 | 25.04 |
| ATOM | 712 | CA | GLY | 1549 | -6.643 | 1.855 | 15.516 | 1.00 | 25.47 |
| ATOM | 713 | C | GLY | 1549 | -6.417 | 3.336 | 15.367 | 1.00 | 26.23 |
| ATOM | 714 | O | GLY | 1549 | -5.267 | 3.781 | 15.287 | 1.00 | 28.41 |
| ATOM | 715 | N | ALA | 1550 | -7.501 | 4.104 | 15.349 | 1.00 | 25.49 |
| ATOM | 717 | CA | ALA | 1550 | -7.408 | 5.550 | 15.198 | 1.00 | 24.81 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 718 | CB | ALA | 1550 | -7.176 | 5.913 | 13.724 | 1.00 | 21.79 |
| ATOM | 719 | C | ALA | 1550 | -8.645 | 6.271 | 15.691 | 1.00 | 25.51 |
| ATOM | 720 | O | ALA | 1550 | -9.738 | 5.702 | 15.726 | 1.00 | 24.09 |
| ATOM | 721 | N | CYS | 1551 | -8.440 | 7.527 | 16.080 | 1.00 | 24.90 |
| ATOM | 723 | CA | CYS | 1551 | -9.492 | 8.438 | 16.511 | 1.00 | 26.80 |
| ATOM | 724 | CB | CYS | 1551 | -9.243 | 8.932 | 17.944 | 1.00 | 26.32 |
| ATOM | 725 | SG | CYS | 1551 | -9.333 | 7.655 | 19.223 | 1.00 | 32.31 |
| ATOM | 726 | C | CYS | 1551 | -9.341 | 9.585 | 15.502 | 1.00 | 28.31 |
| ATOM | 727 | O | CYS | 1551 | -8.361 | 10.338 | 15.537 | 1.00 | 28.42 |
| ATOM | 728 | N | THR | 1552 | -10.261 | 9.660 | 14.547 | 1.00 | 28.38 |
| ATOM | 730 | CA | THR | 1552 | -10.198 | 10.671 | 13.498 | 1.00 | 31.26 |
| ATOM | 731 | CB | THR | 1552 | -10.159 | 9.977 | 12.095 | 1.00 | 30.07 |
| ATOM | 732 | OG1 | THR | 1552 | -11.406 | 9.309 | 11.836 | 1.00 | 29.64 |
| ATOM | 734 | CG2 | THR | 1552 | -9.044 | 8.945 | 12.053 | 1.00 | 28.65 |
| ATOM | 735 | C | THR | 1552 | -11.355 | 11.662 | 13.509 | 1.00 | 33.31 |
| ATOM | 736 | O | THR | 1552 | -11.295 | 12.722 | 12.874 | 1.00 | 31.94 |
| ATOM | 737 | N | GLN | 1553 | -12.420 | 11.309 | 14.214 | 1.00 | 36.09 |
| ATOM | 739 | CA | GLN | 1553 | -13.598 | 12.158 | 14.245 | 1.00 | 39.26 |
| ATOM | 740 | CB | GLN | 1553 | -14.864 | 11.299 | 14.145 | 1.00 | 36.61 |
| ATOM | 741 | CG | GLN | 1553 | -14.932 | 10.436 | 12.881 | 1.00 | 37.72 |
| ATOM | 742 | CD | GLN | 1553 | -14.762 | 11.247 | 11.601 | 1.00 | 38.41 |
| ATOM | 743 | OE1 | GLN | 1553 | -15.491 | 12.210 | 11.363 | 1.00 | 37.88 |
| ATOM | 744 | NE2 | GLN | 1553 | -13.798 | 10.858 | 10.770 | 1.00 | 37.67 |
| ATOM | 747 | C | GLN | 1553 | -13.671 | 13.079 | 15.451 | 1.00 | 41.28 |
| ATOM | 748 | O | GLN | 1553 | -13.150 | 12.758 | 16.513 | 1.00 | 41.37 |
| ATOM | 749 | N | ASP | 1554 | -14.282 | 14.246 | 15.243 | 1.00 | 44.93 |
| ATOM | 751 | CA | ASP | 1554 | -14.487 | 15.254 | 16.281 | 1.00 | 48.05 |
| ATOM | 752 | CB | ASP | 1554 | -15.828 | 15.009 | 16.975 | 1.00 | 50.80 |
| ATOM | 753 | CG | ASP | 1554 | -17.007 | 15.281 | 16.067 | 1.00 | 56.88 |
| ATOM | 754 | OD1 | ASP | 1554 | -17.921 | 16.019 | 16.491 | 1.00 | 63.89 |
| ATOM | 755 | OD2 | ASP | 1554 | -17.016 | 14.776 | 14.925 | 1.00 | 58.98 |
| ATOM | 756 | C | ASP | 1554 | -13.367 | 15.366 | 17.316 | 1.00 | 48.04 |
| ATOM | 757 | O | ASP | 1554 | -13.556 | 15.056 | 18.502 | 1.00 | 48.73 |
| ATOM | 758 | N | GLY | 1555 | -12.205 | 15.819 | 16.860 | 1.00 | 44.30 |
| ATOM | 760 | CA | GLY | 1555 | -11.080 | 15.960 | 17.756 | 1.00 | 42.32 |
| ATOM | 761 | C | GLY | 1555 | -9.761 | 15.713 | 17.052 | 1.00 | 40.69 |
| ATOM | 762 | O | GLY | 1555 | -9.740 | 15.465 | 15.848 | 1.00 | 40.71 |
| ATOM | 763 | N | PRO | 1556 | -8.644 | 15.776 | 17.782 | 1.00 | 39.49 |
| ATOM | 764 | CD | PRO | 1556 | -8.585 | 15.983 | 19.235 | 1.00 | 40.36 |
| ATOM | 765 | CA | PRO | 1556 | -7.298 | 15.566 | 17.250 | 1.00 | 38.37 |
| ATOM | 766 | CB | PRO | 1556 | -6.405 | 15.771 | 18.470 | 1.00 | 38.47 |
| ATOM | 767 | CG | PRO | 1556 | -7.226 | 16.573 | 19.388 | 1.00 | 41.77 |
| ATOM | 768 | C | PRO | 1556 | -7.140 | 14.154 | 16.746 | 1.00 | 36.92 |
| ATOM | 769 | O | PRO | 1556 | -7.606 | 13.208 | 17.371 | 1.00 | 37.04 |
| ATOM | 770 | N | LEU | 1557 | -6.447 | 14.017 | 15.627 | 1.00 | 36.70 |
| ATOM | 772 | CA | LEU | 1557 | -6.201 | 12.719 | 15.037 | 1.00 | 34.81 |
| ATOM | 773 | CB | LEU | 1557 | -5.528 | 12.885 | 13.664 | 1.00 | 32.49 |
| ATOM | 774 | CG | LEU | 1557 | -5.004 | 11.623 | 12.954 | 1.00 | 30.83 |
| ATOM | 775 | CD1 | LEU | 1557 | -6.146 | 10.655 | 12.664 | 1.00 | 26.28 |
| ATOM | 776 | CD2 | LEU | 1557 | -4.283 | 12.014 | 11.672 | 1.00 | 25.55 |
| ATOM | 777 | C | LEU | 1557 | -5.290 | 11.925 | 15.961 | 1.00 | 33.63 |
| ATOM | 778 | O | LEU | 1557 | -4.229 | 12.410 | 16.369 | 1.00 | 33.62 |
| ATOM | 779 | N | TYR | 1558 | -5.718 | 10.724 | 16.319 | 1.00 | 31.97 |
| ATOM | 781 | CA | TYR | 1558 | -4.902 | 9.863 | 17.147 | 1.00 | 31.81 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 782 | CB | TYR | 1558 | -5.614 | 9.500 | 18.462 | 1.00 | 33.55 |
| ATOM | 783 | CG | TYR | 1558 | -5.710 | 10.638 | 19.461 | 1.00 | 35.33 |
| ATOM | 784 | CD1 | TYR | 1558 | -6.644 | 10.608 | 20.499 | 1.00 | 35.68 |
| ATOM | 785 | CE1 | TYR | 1558 | -6.757 | 11.670 | 21.394 | 1.00 | 38.60 |
| ATOM | 786 | CD2 | TYR | 1558 | -4.883 | 11.759 | 19.349 | 1.00 | 38.62 |
| ATOM | 787 | CE2 | TYR | 1558 | -4.985 | 12.824 | 20.235 | 1.00 | 40.33 |
| ATOM | 788 | CZ | TYR | 1558 | -5.924 | 12.781 | 21.254 | 1.00 | 41.70 |
| ATOM | 789 | OH | TYR | 1558 | -6.040 | 13.867 | 22.104 | 1.00 | 42.66 |
| ATOM | 791 | C | TYR | 1558 | -4.607 | 8.604 | 16.345 | 1.00 | 31.08 |
| ATOM | 792 | O | TYR | 1558 | -5.527 | 7.937 | 15.857 | 1.00 | 31.28 |
| ATOM | 793 | N | VAL | 1559 | -3.328 | 8.336 | 16.116 | 1.00 | 28.34 |
| ATOM | 795 | CA | VAL | 1559 | -2.934 | 7.132 | 15.403 | 1.00 | 26.39 |
| ATOM | 796 | CB | VAL | 1559 | -1.830 | 7.401 | 14.364 | 1.00 | 29.17 |
| ATOM | 797 | CG1 | VAL | 1559 | -1.463 | 6.103 | 13.648 | 1.00 | 26.25 |
| ATOM | 798 | CG2 | VAL | 1559 | -2.297 | 8.461 | 13.360 | 1.00 | 29.56 |
| ATOM | 799 | C | VAL | 1559 | -2.411 | 6.226 | 16.498 | 1.00 | 25.14 |
| ATOM | 800 | O | VAL | 1559 | -1.396 | 6.522 | 17.120 | 1.00 | 28.04 |
| ATOM | 801 | N | ILE | 1560 | -3.164 | 5.171 | 16.783 | 1.00 | 25.28 |
| ATOM | 803 | CA | ILE | 1560 | -2.832 | 4.208 | 17.831 | 1.00 | 24.81 |
| ATOM | 804 | CB | ILE | 1560 | -4.133 | 3.669 | 18.496 | 1.00 | 24.63 |
| ATOM | 805 | CG2 | ILE | 1560 | -3.790 | 2.812 | 19.728 | 1.00 | 20.93 |
| ATOM | 806 | CG1 | ILE | 1560 | -5.044 | 4.854 | 18.869 | 1.00 | 22.94 |
| ATOM | 807 | CD1 | ILE | 1560 | -6.499 | 4.502 | 19.028 | 1.00 | 25.34 |
| ATOM | 808 | C | ILE | 1560 | -1.994 | 3.051 | 17.286 | 1.00 | 26.38 |
| ATOM | 809 | O | ILE | 1560 | -2.429 | 2.301 | 16.398 | 1.00 | 26.14 |
| ATOM | 810 | N | VAL | 1561 | -0.782 | 2.911 | 17.809 | 1.00 | 27.31 |
| ATOM | 812 | CA | VAL | 1561 | 0.112 | 1.852 | 17.359 | 1.00 | 27.32 |
| ATOM | 813 | CB | VAL | 1561 | 1.309 | 2.435 | 16.527 | 1.00 | 25.01 |
| ATOM | 814 | CG1 | VAL | 1561 | 0.785 | 3.220 | 15.338 | 1.00 | 19.39 |
| ATOM | 815 | CG2 | VAL | 1561 | 2.170 | 3.340 | 17.397 | 1.00 | 26.08 |
| ATOM | 816 | C | VAL | 1561 | 0.615 | 1.029 | 18.548 | 1.00 | 25.89 |
| ATOM | 817 | O | VAL | 1561 | 0.364 | 1.373 | 19.713 | 1.00 | 25.64 |
| ATOM | 818 | N | GLU | 1562 | 1.288 | -0.076 | 18.250 | 1.00 | 24.49 |
| ATOM | 820 | CA | GLU | 1562 | 1.806 | -0.949 | 19.284 | 1.00 | 25.00 |
| ATOM | 821 | CB | GLU | 1562 | 2.357 | -2.231 | 18.677 | 1.00 | 23.69 |
| ATOM | 822 | CG | GLU | 1562 | 1.272 | -3.170 | 18.219 | 1.00 | 24.29 |
| ATOM | 823 | CD | GLU | 1562 | 1.814 | -4.393 | 17.514 | 1.00 | 27.65 |
| ATOM | 824 | OE1 | GLU | 1562 | 1.218 | -5.480 | 17.649 | 1.00 | 29.50 |
| ATOM | 825 | OE2 | GLU | 1562 | 2.832 | -4.270 | 16.807 | 1.00 | 32.34 |
| ATOM | 826 | C | GLU | 1562 | 2.840 | -0.279 | 20.170 | 1.00 | 27.27 |
| ATOM | 827 | O | GLU | 1562 | 3.596 | 0.576 | 19.729 | 1.00 | 26.18 |
| ATOM | 828 | N | TYR | 1563 | 2.822 | -0.663 | 21.441 | 1.00 | 30.39 |
| ATOM | 830 | CA | TYR | 1563 | 3.715 | -0.121 | 22.454 | 1.00 | 32.48 |
| ATOM | 831 | CB | TYR | 1563 | 2.932 | 0.132 | 23.750 | 1.00 | 33.91 |
| ATOM | 832 | CG | TYR | 1563 | 3.788 | 0.535 | 24.928 | 1.00 | 34.93 |
| ATOM | 833 | CD1 | TYR | 1563 | 4.606 | 1.664 | 24.871 | 1.00 | 34.50 |
| ATOM | 834 | CE1 | TYR | 1563 | 5.374 | 2.051 | 25.967 | 1.00 | 37.77 |
| ATOM | 835 | CD2 | TYR | 1563 | 3.758 | -0.201 | 26.108 | 1.00 | 33.54 |
| ATOM | 836 | CE2 | TYR | 1563 | 4.519 | 0.171 | 27.205 | 1.00 | 34.94 |
| ATOM | 837 | CZ | TYR | 1563 | 5.321 | 1.296 | 27.128 | 1.00 | 37.22 |
| ATOM | 838 | OH | TYR | 1563 | 6.087 | 1.648 | 28.206 | 1.00 | 45.36 |
| ATOM | 840 | C | TYR | 1563 | 4.896 | -1.039 | 22.730 | 1.00 | 31.53 |
| ATOM | 841 | O | TYR | 1563 | 4.737 | -2.252 | 22.895 | 1.00 | 30.43 |
| ATOM | 842 | N | ALA | 1564 | 6.082 | -0.444 | 22.761 | 1.00 | 32.28 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 844 | CA | ALA | 1564 | 7.326 | -1.167 | 23.026 | 1.00 | 32.59 |
| ATOM | 845 | CB | ALA | 1564 | 8.308 | -0.957 | 21.863 | 1.00 | 30.11 |
| ATOM | 846 | C | ALA | 1564 | 7.897 | -0.608 | 24.334 | 1.00 | 31.81 |
| ATOM | 847 | O | ALA | 1564 | 8.563 | 0.427 | 24.345 | 1.00 | 34.11 |
| ATOM | 848 | N | SER | 1565 | 7.619 | -1.296 | 25.434 | 1.00 | 34.09 |
| ATOM | 850 | CA | SER | 1565 | 8.039 | -0.853 | 26.763 | 1.00 | 35.05 |
| ATOM | 851 | CB | SER | 1565 | 7.400 | -1.725 | 27.829 | 1.00 | 30.13 |
| ATOM | 852 | OG | SER | 1565 | 7.689 | -3.084 | 27.579 | 1.00 | 38.17 |
| ATOM | 854 | C | SER | 1565 | 9.526 | -0.769 | 27.041 | 1.00 | 35.03 |
| ATOM | 855 | O | SER | 1565 | 9.947 | -0.001 | 27.902 | 1.00 | 37.12 |
| ATOM | 856 | N | LYS | 1566 | 10.321 | -1.557 | 26.330 | 1.00 | 34.55 |
| ATOM | 858 | CA | LYS | 1566 | 11.756 | -1.559 | 26.562 | 1.00 | 33.48 |
| ATOM | 859 | CB | LYS | 1566 | 12.291 | -2.990 | 26.508 | 1.00 | 31.90 |
| ATOM | 860 | CG | LYS | 1566 | 11.674 | -3.865 | 27.586 | 1.00 | 28.63 |
| ATOM | 861 | CD | LYS | 1566 | 12.162 | -5.287 | 27.508 | 1.00 | 34.97 |
| ATOM | 862 | CE | LYS | 1566 | 11.763 | -6.042 | 28.761 | 1.00 | 36.82 |
| ATOM | 863 | NZ | LYS | 1566 | 12.288 | -7.433 | 28.748 | 1.00 | 41.32 |
| ATOM | 867 | C | LYS | 1566 | 12.567 | -0.613 | 25.691 | 1.00 | 34.98 |
| ATOM | 868 | O | LYS | 1566 | 13.785 | -0.740 | 25.607 | 1.00 | 38.03 |
| ATOM | 869 | N | GLY | 1567 | 11.892 | 0.338 | 25.049 | 1.00 | 36.00 |
| ATOM | 871 | CA | GLY | 1567 | 12.582 | 1.322 | 24.222 | 1.00 | 34.14 |
| ATOM | 872 | C | GLY | 1567 | 13.245 | 0.864 | 22.933 | 1.00 | 32.01 |
| ATOM | 873 | O | GLY | 1567 | 12.975 | -0.222 | 22.439 | 1.00 | 31.95 |
| ATOM | 874 | N | ASN | 1568 | 14.091 | 1.719 | 22.360 | 1.00 | 33.51 |
| ATOM | 876 | CA | ASN | 1568 | 14.774 | 1.375 | 21.121 | 1.00 | 34.20 |
| ATOM | 877 | CB | ASN | 1568 | 15.203 | 2.627 | 20.332 | 1.00 | 34.07 |
| ATOM | 878 | CG | ASN | 1568 | 16.420 | 3.321 | 20.910 | 1.00 | 35.09 |
| ATOM | 879 | OD1 | ASN | 1568 | 17.453 | 2.709 | 21.156 | 1.00 | 34.36 |
| ATOM | 880 | ND2 | ASN | 1568 | 16.317 | 4.624 | 21.066 | 1.00 | 38.38 |
| ATOM | 883 | C | ASN | 1568 | 15.927 | 0.401 | 21.325 | 1.00 | 33.38 |
| ATOM | 884 | O | ASN | 1568 | 16.490 | 0.315 | 22.414 | 1.00 | 34.93 |
| ATOM | 885 | N | LEU | 1569 | 16.276 | -0.317 | 20.263 | 1.00 | 31.11 |
| ATOM | 887 | CA | LEU | 1569 | 17.333 | -1.316 | 20.298 | 1.00 | 30.44 |
| ATOM | 888 | CB | LEU | 1569 | 17.437 | -2.008 | 18.928 | 1.00 | 29.46 |
| ATOM | 889 | CG | LEU | 1569 | 18.438 | -3.148 | 18.741 | 1.00 | 29.01 |
| ATOM | 890 | CD1 | LEU | 1569 | 18.285 | -4.219 | 19.840 | 1.00 | 28.81 |
| ATOM | 891 | CD2 | LEU | 1569 | 18.263 | -3.740 | 17.338 | 1.00 | 26.62 |
| ATOM | 892 | C | LEU | 1569 | 18.706 | -0.805 | 20.762 | 1.00 | 30.16 |
| ATOM | 893 | O | LEU | 1569 | 19.400 | -1.501 | 21.496 | 1.00 | 27.32 |
| ATOM | 894 | N | ARG | 1570 | 19.097 | 0.396 | 20.344 | 1.00 | 30.74 |
| ATOM | 896 | CA | ARG | 1570 | 20.386 | 0.951 | 20.758 | 1.00 | 33.72 |
| ATOM | 897 | CB | ARG | 1570 | 20.597 | 2.349 | 20.160 | 1.00 | 32.82 |
| ATOM | 898 | CG | ARG | 1570 | 21.873 | 3.009 | 20.662 | 1.00 | 36.90 |
| ATOM | 899 | CD | ARG | 1570 | 21.966 | 4.481 | 20.332 | 1.00 | 39.32 |
| ATOM | 900 | NE | ARG | 1570 | 20.749 | 5.222 | 20.664 | 1.00 | 50.32 |
| ATOM | 902 | CZ | ARG | 1570 | 20.376 | 5.600 | 21.889 | 1.00 | 51.90 |
| ATOM | 903 | NH1 | ARG | 1570 | 21.118 | 5.316 | 22.960 | 1.00 | 50.15 |
| ATOM | 906 | NH2 | ARG | 1570 | 19.246 | 6.284 | 22.033 | 1.00 | 53.67 |
| ATOM | 909 | C | ARG | 1570 | 20.434 | 1.022 | 22.298 | 1.00 | 35.75 |
| ATOM | 910 | O | ARG | 1570 | 21.324 | 0.444 | 22.939 | 1.00 | 35.67 |
| ATOM | 911 | N | GLU | 1571 | 19.444 | 1.695 | 22.880 | 1.00 | 35.56 |
| ATOM | 913 | CA | GLU | 1571 | 19.331 | 1.835 | 24.328 | 1.00 | 36.50 |
| ATOM | 914 | CB | GLU | 1571 | 18.055 | 2.607 | 24.667 | 1.00 | 39.08 |
| ATOM | 915 | CG | GLU | 1571 | 18.061 | 4.056 | 24.208 | 1.00 | 46.75 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 916 | CD | GLU | 1571 | 16.694 | 4.721 | 24.311 | 1.00 | 51.36 |
| ATOM | 917 | OE1 | GLU | 1571 | 15.676 | 3.996 | 24.417 | 1.00 | 55.22 |
| ATOM | 918 | OE2 | GLU | 1571 | 16.635 | 5.972 | 24.267 | 1.00 | 53.59 |
| ATOM | 919 | C | GLU | 1571 | 19.314 | 0.469 | 25.022 | 1.00 | 34.82 |
| ATOM | 920 | O | GLU | 1571 | 20.018 | 0.242 | 26.013 | 1.00 | 35.05 |
| ATOM | 921 | N | TYR | 1572 | 18.520 | -0.441 | 24.469 | 1.00 | 33.35 |
| ATOM | 923 | CA | TYR | 1572 | 18.366 | -1.796 | 24.986 | 1.00 | 31.83 |
| ATOM | 924 | CB | TYR | 1572 | 17.365 | -2.544 | 24.102 | 1.00 | 30.77 |
| ATOM | 925 | CG | TYR | 1572 | 17.170 | -4.008 | 24.408 | 1.00 | 28.50 |
| ATOM | 926 | CD1 | TYR | 1572 | 16.193 | -4.420 | 25.313 | 1.00 | 30.48 |
| ATOM | 927 | CE1 | TYR | 1572 | 15.977 | -5.760 | 25.574 | 1.00 | 30.97 |
| ATOM | 928 | CD2 | TYR | 1572 | 17.933 | -4.985 | 23.772 | 1.00 | 26.14 |
| ATOM | 929 | CE2 | TYR | 1572 | 17.725 | -6.329 | 24.027 | 1.00 | 26.21 |
| ATOM | 930 | CZ | TYR | 1572 | 16.742 | -6.708 | 24.935 | 1.00 | 30.30 |
| ATOM | 931 | OH | TYR | 1572 | 16.518 | -8.041 | 25.214 | 1.00 | 33.52 |
| ATOM | 933 | C | TYR | 1572 | 19.692 | -2.556 | 25.044 | 1.00 | 34.83 |
| ATOM | 934 | O | TYR | 1572 | 19.959 | -3.308 | 25.992 | 1.00 | 34.93 |
| ATOM | 935 | N | LEU | 1573 | 20.517 | -2.370 | 24.020 | 1.00 | 34.34 |
| ATOM | 937 | CA | LEU | 1573 | 21.803 | -3.053 | 23.961 | 1.00 | 35.38 |
| ATOM | 938 | CB | LEU | 1573 | 22.357 | -3.027 | 22.531 | 1.00 | 32.71 |
| ATOM | 939 | CG | LEU | 1573 | 21.669 | -3.891 | 21.464 | 1.00 | 29.16 |
| ATOM | 940 | CD1 | LEU | 1573 | 22.161 | -3.503 | 20.087 | 1.00 | 26.98 |
| ATOM | 941 | CD2 | LEU | 1573 | 21.932 | -5.351 | 21.710 | 1.00 | 28.85 |
| ATOM | 942 | C | LEU | 1573 | 22.799 | -2.420 | 24.933 | 1.00 | 37.54 |
| ATOM | 943 | O | LEU | 1573 | 23.511 | -3.123 | 25.659 | 1.00 | 36.67 |
| ATOM | 944 | N | GLN | 1574 | 22.814 | -1.092 | 24.969 | 1.00 | 37.90 |
| ATOM | 946 | CA | GLN | 1574 | 23.729 | -0.368 | 25.838 | 1.00 | 39.77 |
| ATOM | 947 | CB | GLN | 1574 | 23.624 | 1.138 | 25.572 | 1.00 | 40.09 |
| ATOM | 948 | CG | GLN | 1574 | 24.208 | 1.549 | 24.217 | 1.00 | 42.28 |
| ATOM | 949 | CD | GLN | 1574 | 24.030 | 3.018 | 23.896 | 1.00 | 44.28 |
| ATOM | 950 | OE1 | GLN | 1574 | 23.362 | 3.755 | 24.615 | 1.00 | 47.55 |
| ATOM | 951 | NE2 | GLN | 1574 | 24.613 | 3.448 | 22.790 | 1.00 | 46.09 |
| ATOM | 954 | C | GLN | 1574 | 23.490 | -0.697 | 27.310 | 1.00 | 40.75 |
| ATOM | 955 | O | GLN | 1574 | 24.440 | -0.939 | 28.059 | 1.00 | 41.29 |
| ATOM | 956 | N | ALA | 1575 | 22.220 | -0.783 | 27.696 | 1.00 | 40.10 |
| ATOM | 958 | CA | ALA | 1575 | 21.842 | -1.088 | 29.069 | 1.00 | 38.81 |
| ATOM | 959 | CB | ALA | 1575 | 20.349 | -0.819 | 29.273 | 1.00 | 35.69 |
| ATOM | 960 | C | ALA | 1575 | 22.192 | -2.514 | 29.503 | 1.00 | 40.63 |
| ATOM | 961 | O | ALA | 1575 | 22.098 | -2.843 | 30.690 | 1.00 | 43.39 |
| ATOM | 962 | N | ARG | 1576 | 22.602 | -3.357 | 28.561 | 1.00 | 38.39 |
| ATOM | 964 | CA | ARG | 1576 | 22.945 | -4.729 | 28.896 | 1.00 | 37.69 |
| ATOM | 965 | CB | ARG | 1576 | 22.034 | -5.689 | 28.137 | 1.00 | 38.16 |
| ATOM | 966 | CG | ARG | 1576 | 20.594 | -5.547 | 28.589 | 1.00 | 37.89 |
| ATOM | 967 | CD | ARG | 1576 | 19.622 | -6.281 | 27.711 | 1.00 | 37.36 |
| ATOM | 968 | NE | ARG | 1576 | 18.267 | -6.255 | 28.265 | 1.00 | 34.99 |
| ATOM | 970 | CZ | ARG | 1576 | 17.565 | -5.150 | 28.484 | 1.00 | 36.94 |
| ATOM | 971 | NH1 | ARG | 1576 | 18.083 | -3.960 | 28.209 | 1.00 | 36.18 |
| ATOM | 974 | NH2 | ARG | 1576 | 16.310 | -5.237 | 28.909 | 1.00 | 40.93 |
| ATOM | 977 | C | ARG | 1576 | 24.413 | -5.073 | 28.704 | 1.00 | 38.93 |
| ATOM | 978 | O | ARG | 1576 | 24.801 | -6.249 | 28.699 | 1.00 | 39.75 |
| ATOM | 979 | N | ARG | 1577 | 25.233 | -4.036 | 28.570 | 1.00 | 39.21 |
| ATOM | 981 | CA | ARG | 1577 | 26.671 | -4.196 | 28.413 | 1.00 | 38.97 |
| ATOM | 982 | CB | ARG | 1577 | 27.307 | -2.870 | 28.000 | 1.00 | 36.06 |
| ATOM | 983 | CG | ARG | 1577 | 26.992 | -2.408 | 26.610 | 1.00 | 36.41 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 984 | CD | ARG | 1577 | 27.695 | -1.094 | 26.337 | 1.00 | 36.17 |
| ATOM | 985 | NE | ARG | 1577 | 27.776 | -0.806 | 24.907 | 1.00 | 38.45 |
| ATOM | 987 | CZ | ARG | 1577 | 28.284 | 0.309 | 24.387 | 1.00 | 39.00 |
| ATOM | 988 | NH1 | ARG | 1577 | 28.764 | 1.262 | 25.175 | 1.00 | 38.88 |
| ATOM | 991 | NH2 | ARG | 1577 | 28.311 | 0.469 | 23.071 | 1.00 | 37.76 |
| ATOM | 994 | C | ARG | 1577 | 27.247 | -4.571 | 29.772 | 1.00 | 40.59 |
| ATOM | 995 | O | ARG | 1577 | 26.680 | -4.217 | 30.800 | 1.00 | 38.52 |
| ATOM | 996 | N | PRO | 1578 | 28.358 | -5.327 | 29.796 | 1.00 | 43.19 |
| ATOM | 997 | CD | PRO | 1578 | 29.077 | -5.980 | 28.692 | 1.00 | 44.84 |
| ATOM | 998 | CA | PRO | 1578 | 28.952 | -5.692 | 31.088 | 1.00 | 45.06 |
| ATOM | 999 | CB | PRO | 1578 | 30.065 | -6.673 | 30.689 | 1.00 | 44.86 |
| ATOM | 1000 | CG | PRO | 1578 | 30.431 | -6.229 | 29.308 | 1.00 | 44.56 |
| ATOM | 1001 | C | PRO | 1578 | 29.513 | -4.420 | 31.734 | 1.00 | 44.93 |
| ATOM | 1002 | O | PRO | 1578 | 29.809 | -3.439 | 31.043 | 1.00 | 43.13 |
| ATOM | 1003 | N | PRO | 1579 | 29.649 | -4.414 | 33.067 | 1.00 | 47.61 |
| ATOM | 1004 | CD | PRO | 1579 | 29.315 | -5.492 | 34.012 | 1.00 | 48.39 |
| ATOM | 1005 | CA | PRO | 1579 | 30.173 | -3.247 | 33.784 | 1.00 | 48.74 |
| ATOM | 1006 | CB | PRO | 1579 | 30.138 | -3.706 | 35.238 | 1.00 | 49.73 |
| ATOM | 1007 | CG | PRO | 1579 | 29.027 | -4.711 | 35.259 | 1.00 | 49.21 |
| ATOM | 1008 | C | PRO | 1579 | 31.591 | -2.888 | 33.357 | 1.00 | 49.67 |
| ATOM | 1009 | O | PRO | 1579 | 32.483 | -3.733 | 33.361 | 1.00 | 52.07 |
| ATOM | 1010 | N | GLU | 1592 | 19.165 | -5.411 | 32.444 | 1.00 | 64.83 |
| ATOM | 1012 | CA | GLU | 1592 | 20.603 | -5.147 | 32.491 | 1.00 | 64.82 |
| ATOM | 1013 | CB | GLU | 1592 | 20.969 | -4.421 | 33.784 | 1.00 | 67.61 |
| ATOM | 1014 | C | GLU | 1592 | 21.448 | -6.413 | 32.335 | 1.00 | 63.99 |
| ATOM | 1015 | O | GLU | 1592 | 22.653 | -6.336 | 32.098 | 1.00 | 65.67 |
| ATOM | 1016 | N | GLU | 1593 | 20.821 | -7.575 | 32.485 | 1.00 | 62.41 |
| ATOM | 1018 | CA | GLU | 1593 | 21.534 | -8.844 | 32.342 | 1.00 | 61.23 |
| ATOM | 1019 | CB | GLU | 1593 | 20.595 | -10.017 | 32.600 | 1.00 | 61.20 |
| ATOM | 1020 | C | GLU | 1593 | 22.141 | -8.953 | 30.944 | 1.00 | 59.26 |
| ATOM | 1021 | O | GLU | 1593 | 21.494 | -8.631 | 29.945 | 1.00 | 59.84 |
| ATOM | 1022 | N | GLN | 1594 | 23.388 | -9.405 | 30.888 | 1.00 | 57.94 |
| ATOM | 1024 | CA | GLN | 1594 | 24.101 | -9.558 | 29.625 | 1.00 | 54.91 |
| ATOM | 1025 | CB | GLN | 1594 | 25.501 | -10.141 | 29.865 | 1.00 | 55.13 |
| ATOM | 1026 | CG | GLN | 1594 | 26.439 | -9.252 | 30.679 | 1.00 | 56.93 |
| ATOM | 1027 | CD | GLN | 1594 | 27.682 | -9.997 | 31.180 | 1.00 | 59.60 |
| ATOM | 1028 | OE1 | GLN | 1594 | 28.241 | -10.858 | 30.488 | 1.00 | 58.45 |
| ATOM | 1029 | NE2 | GLN | 1594 | 28.117 | -9.662 | 32.393 | 1.00 | 58.95 |
| ATOM | 1032 | C | GLN | 1594 | 23.331 | -10.438 | 28.640 | 1.00 | 52.30 |
| ATOM | 1033 | O | GLN | 1594 | 22.637 | -11.389 | 29.025 | 1.00 | 52.03 |
| ATOM | 1034 | N | LEU | 1595 | 23.438 | -10.091 | 27.366 | 1.00 | 49.60 |
| ATOM | 1036 | CA | LEU | 1595 | 22.782 | -10.836 | 26.308 | 1.00 | 45.16 |
| ATOM | 1037 | CB | LEU | 1595 | 22.459 | -9.907 | 25.135 | 1.00 | 41.36 |
| ATOM | 1038 | CG | LEU | 1595 | 21.463 | -8.815 | 25.523 | 1.00 | 39.43 |
| ATOM | 1039 | CD1 | LEU | 1595 | 21.617 | -7.583 | 24.644 | 1.00 | 36.21 |
| ATOM | 1040 | CD2 | LEU | 1595 | 20.060 | -9.389 | 25.480 | 1.00 | 34.91 |
| ATOM | 1041 | C | LEU | 1595 | 23.747 | -11.900 | 25.858 | 1.00 | 43.30 |
| ATOM | 1042 | O | LEU | 1595 | 24.953 | -11.675 | 25.841 | 1.00 | 43.62 |
| ATOM | 1043 | N | SER | 1596 | 23.230 | -13.081 | 25.553 | 1.00 | 42.92 |
| ATOM | 1045 | CA | SER | 1596 | 24.085 | -14.150 | 25.077 | 1.00 | 41.86 |
| ATOM | 1046 | CB | SER | 1596 | 23.410 | -15.502 | 25.298 | 1.00 | 40.86 |
| ATOM | 1047 | OG | SER | 1596 | 22.188 | -15.596 | 24.595 | 1.00 | 37.88 |
| ATOM | 1049 | C | SER | 1596 | 24.322 | -13.914 | 23.587 | 1.00 | 41.59 |
| ATOM | 1050 | O | SER | 1596 | 23.657 | -13.077 | 22.966 | 1.00 | 41.94 |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1051 | N | SER | 1597 | 25.275 | -14.637 | 23.018 | 1.00 | 39.60 | |
| ATOM | 1053 | CA | SER | 1597 | 25.557 | -14.518 | 21.603 | 1.00 | 39.74 | |
| ATOM | 1054 | CB | SER | 1597 | 26.729 | -15.409 | 21.223 | 1.00 | 41.38 | |
| ATOM | 1055 | OG | SER | 1597 | 27.824 | -15.147 | 22.077 | 1.00 | 50.59 | |
| ATOM | 1057 | C | SER | 1597 | 24.315 | -14.921 | 20.818 | 1.00 | 38.16 | |
| ATOM | 1058 | O | SER | 1597 | 24.036 | -14.353 | 19.769 | 1.00 | 38.03 | |
| ATOM | 1059 | N | LYS | 1598 | 23.560 | -15.891 | 21.327 | 1.00 | 36.40 | |
| ATOM | 1061 | CA | LYS | 1598 | 22.362 | -16.312 | 20.634 | 1.00 | 35.97 | |
| ATOM | 1062 | CB | LYS | 1598 | 21.791 | -17.594 | 21.228 | 1.00 | 36.69 | |
| ATOM | 1063 | CG | LYS | 1598 | 20.989 | -18.402 | 20.198 | 1.00 | 40.42 | |
| ATOM | 1064 | CD | LYS | 1598 | 20.164 | -19.499 | 20.838 | 1.00 | 40.37 | |
| ATOM | 1065 | CE | LYS | 1598 | 19.792 | -20.572 | 19.829 | 1.00 | 46.34 | |
| ATOM | 1066 | NZ | LYS | 1598 | 20.993 | -21.338 | 19.362 | 1.00 | 45.29 | |
| ATOM | 1070 | C | LYS | 1598 | 21.324 | -15.194 | 20.696 | 1.00 | 37.49 | |
| ATOM | 1071 | O | LYS | 1598 | 20.567 | -14.983 | 19.738 | 1.00 | 38.10 | |
| ATOM | 1072 | N | ASP | 1599 | 21.316 | -14.458 | 21.807 | 1.00 | 35.21 | |
| ATOM | 1074 | CA | ASP | 1599 | 20.380 | -13.352 | 21.983 | 1.00 | 34.02 | |
| ATOM | 1075 | CB | ASP | 1599 | 20.556 | -12.686 | 23.346 | 1.00 | 37.78 | |
| ATOM | 1076 | CG | ASP | 1599 | 19.970 | -13.493 | 24.483 | 1.00 | 40.05 | |
| ATOM | 1077 | OD1 | ASP | 1599 | 20.270 | -13.143 | 25.642 | 1.00 | 42.73 | |
| ATOM | 1078 | OD2 | ASP | 1599 | 19.204 | -14.450 | 24.235 | 1.00 | 42.39 | |
| ATOM | 1079 | C | ASP | 1599 | 20.633 | -12.306 | 20.922 | 1.00 | 32.84 | |
| ATOM | 1080 | O | ASP | 1599 | 19.694 | -11.779 | 20.311 | 1.00 | 30.59 | |
| ATOM | 1081 | N | LEU | 1600 | 21.912 | -11.999 | 20.724 | 1.00 | 31.11 | |
| ATOM | 1083 | CA | LEU | 1600 | 22.323 | -10.998 | 19.744 | 1.00 | 32.17 | |
| ATOM | 1084 | CB | LEU | 1600 | 23.823 | -10.722 | 19.875 | 1.00 | 32.30 | |
| ATOM | 1085 | CG | LEU | 1600 | 24.275 | -10.162 | 21.235 | 1.00 | 31.08 | |
| ATOM | 1086 | CD1 | LEU | 1600 | 25.794 | -9.931 | 21.242 | 1.00 | 30.59 | |
| ATOM | 1087 | CD2 | LEU | 1600 | 23.549 | -8.863 | 21.514 | 1.00 | 28.89 | |
| ATOM | 1088 | C | LEU | 1600 | 21.949 | -11.390 | 18.311 | 1.00 | 30.77 | |
| ATOM | 1089 | O | LEU | 1600 | 21.352 | -10.601 | 17.574 | 1.00 | 29.87 | |
| ATOM | 1090 | N | VAL | 1601 | 22.269 | -12.623 | 17.933 | 1.00 | 30.19 | |
| ATOM | 1092 | CA | VAL | 1601 | 21.954 | -13.115 | 16.602 | 1.00 | 29.25 | |
| ATOM | 1093 | CB | VAL | 1601 | 22.593 | -14.497 | 16.349 | 1.00 | 31.27 | |
| ATOM | 1094 | CG1 | VAL | 1601 | 22.355 | -14.936 | 14.914 | 1.00 | 31.60 | |
| ATOM | 1095 | CG2 | VAL | 1601 | 24.093 | -14.434 | 16.622 | 1.00 | 31.91 | |
| ATOM | 1096 | C | VAL | 1601 | 20.438 | -13.181 | 16.405 | 1.00 | 29.06 | |
| ATOM | 1097 | O | VAL | 1601 | 19.946 | -12.914 | 15.310 | 1.00 | 27.71 | |
| ATOM | 1098 | N | SER | 1602 | 19.702 | -13.511 | 17.468 | 1.00 | 29.10 | |
| ATOM | 1100 | CA | SER | 1602 | 18.243 | -13.585 | 17.400 | 1.00 | 29.29 | |
| ATOM | 1101 | CB | SER | 1602 | 17.680 | -14.189 | 18.679 | 1.00 | 30.81 | |
| ATOM | 1102 | OG | SER | 1602 | 16.266 | -14.074 | 18.692 | 1.00 | 35.78 | |
| ATOM | 1104 | C | SER | 1602 | 17.649 | -12.199 | 17.156 | 1.00 | 28.98 | |
| ATOM | 1105 | O | SER | 1602 | 16.662 | -12.039 | 16.426 | 1.00 | 26.82 | |
| ATOM | 1106 | N | CYS | 1603 | 18.274 | -11.202 | 17.765 | 1.00 | 29.06 | |
| ATOM | 1108 | CA | CYS | 1603 | 17.870 | -9.823 | 17.599 | 1.00 | 29.22 | |
| ATOM | 1109 | CB | CYS | 1603 | 18.784 | -8.943 | 18.438 | 1.00 | 29.66 | |
| ATOM | 1110 | SG | CYS | 1603 | 18.575 | -7.212 | 18.103 | 0.50 | 23.69 | PRT1 |
| ATOM | 1111 | C | CYS | 1603 | 17.988 | -9.422 | 16.112 | 1.00 | 29.23 | |
| ATOM | 1112 | O | CYS | 1603 | 17.087 | -8.796 | 15.552 | 1.00 | 27.52 | |
| ATOM | 1113 | N | ALA | 1604 | 19.113 | -9.778 | 15.491 | 1.00 | 27.87 | |
| ATOM | 1115 | CA | ALA | 1604 | 19.376 | -9.484 | 14.077 | 1.00 | 26.37 | |
| ATOM | 1116 | CB | ALA | 1604 | 20.783 | -9.941 | 13.690 | 1.00 | 23.88 | |
| ATOM | 1117 | C | ALA | 1604 | 18.349 | -10.203 | 13.223 | 1.00 | 25.82 | |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1118 | O | ALA | 1604 | 17.788 | -9.631 | 12.289 | 1.00 | 25.84 |
| ATOM | 1119 | N | TYR | 1605 | 18.119 | -11.468 | 13.544 | 1.00 | 25.56 |
| ATOM | 1121 | CA | TYR | 1605 | 17.152 | -12.276 | 12.827 | 1.00 | 27.81 |
| ATOM | 1122 | CB | TYR | 1605 | 17.080 | -13.662 | 13.456 | 1.00 | 26.66 |
| ATOM | 1123 | CG | TYR | 1605 | 15.974 | -14.515 | 12.886 | 1.00 | 30.75 |
| ATOM | 1124 | CD1 | TYR | 1605 | 16.111 | -15.141 | 11.640 | 1.00 | 30.20 |
| ATOM | 1125 | CE1 | TYR | 1605 | 15.088 | -15.944 | 11.126 | 1.00 | 30.03 |
| ATOM | 1126 | CD2 | TYR | 1605 | 14.790 | -14.707 | 13.596 | 1.00 | 30.73 |
| ATOM | 1127 | CE2 | TYR | 1605 | 13.775 | -15.500 | 13.097 | 1.00 | 30.71 |
| ATOM | 1128 | CZ | TYR | 1605 | 13.930 | -16.117 | 11.867 | 1.00 | 30.93 |
| ATOM | 1129 | OH | TYR | 1605 | 12.923 | -16.928 | 11.417 | 1.00 | 32.31 |
| ATOM | 1131 | C | TYR | 1605 | 15.748 | -11.641 | 12.775 | 1.00 | 26.15 |
| ATOM | 1132 | O | TYR | 1605 | 15.147 | -11.551 | 11.702 | 1.00 | 26.64 |
| ATOM | 1133 | N | GLN | 1606 | 15.244 | -11.200 | 13.926 | 1.00 | 25.48 |
| ATOM | 1135 | CA | GLN | 1606 | 13.921 | -10.581 | 14.023 | 1.00 | 26.86 |
| ATOM | 1136 | CB | GLN | 1606 | 13.589 | -10.269 | 15.482 | 1.00 | 26.83 |
| ATOM | 1137 | CG | GLN | 1606 | 13.357 | -11.508 | 16.332 | 1.00 | 25.84 |
| ATOM | 1138 | CD | GLN | 1606 | 13.151 | -11.167 | 17.791 | 1.00 | 30.86 |
| ATOM | 1139 | OE1 | GLN | 1606 | 12.202 | -10.471 | 18.150 | 1.00 | 31.87 |
| ATOM | 1140 | NE2 | GLN | 1606 | 14.056 | -11.631 | 18.640 | 1.00 | 31.67 |
| ATOM | 1143 | C | GLN | 1606 | 13.835 | -9.310 | 13.186 | 1.00 | 27.52 |
| ATOM | 1144 | O | GLN | 1606 | 12.831 | -9.058 | 12.506 | 1.00 | 26.05 |
| ATOM | 1145 | N | VAL | 1607 | 14.904 | -8.523 | 13.216 | 1.00 | 26.68 |
| ATOM | 1147 | CA | VAL | 1607 | 14.963 | -7.301 | 12.435 | 1.00 | 25.66 |
| ATOM | 1148 | CB | VAL | 1607 | 16.225 | -6.485 | 12.787 | 1.00 | 28.50 |
| ATOM | 1149 | CG1 | VAL | 1607 | 16.363 | -5.274 | 11.853 | 1.00 | 26.04 |
| ATOM | 1150 | CG2 | VAL | 1607 | 16.151 | -6.031 | 14.246 | 1.00 | 24.45 |
| ATOM | 1151 | C | VAL | 1607 | 14.934 | -7.641 | 10.938 | 1.00 | 24.89 |
| ATOM | 1152 | O | VAL | 1607 | 14.184 | -7.033 | 10.177 | 1.00 | 25.86 |
| ATOM | 1153 | N | ALA | 1608 | 15.738 | -8.619 | 10.522 | 1.00 | 25.24 |
| ATOM | 1155 | CA | ALA | 1608 | 15.773 | -9.039 | 9.120 | 1.00 | 22.95 |
| ATOM | 1156 | CB | ALA | 1608 | 16.813 | -10.117 | 8.920 | 1.00 | 20.24 |
| ATOM | 1157 | C | ALA | 1608 | 14.383 | -9.541 | 8.679 | 1.00 | 25.71 |
| ATOM | 1158 | O | ALA | 1608 | 13.963 | -9.319 | 7.532 | 1.00 | 27.48 |
| ATOM | 1159 | N | ARG | 1609 | 13.676 | -10.216 | 9.585 | 1.00 | 27.10 |
| ATOM | 1161 | CA | ARG | 1609 | 12.327 | -10.708 | 9.301 | 1.00 | 28.55 |
| ATOM | 1162 | CB | ARG | 1609 | 11.840 | -11.640 | 10.397 | 1.00 | 31.53 |
| ATOM | 1163 | CG | ARG | 1609 | 12.407 | -13.005 | 10.290 | 1.00 | 36.05 |
| ATOM | 1164 | CD | ARG | 1609 | 11.537 | -13.931 | 11.056 | 1.00 | 40.28 |
| ATOM | 1165 | NE | ARG | 1609 | 10.849 | -14.874 | 10.190 | 1.00 | 42.06 |
| ATOM | 1167 | CZ | ARG | 1609 | 9.974 | -15.771 | 10.632 | 1.00 | 42.08 |
| ATOM | 1168 | NH1 | ARG | 1609 | 9.678 | -15.834 | 11.928 | 1.00 | 40.32 |
| ATOM | 1171 | NH2 | ARG | 1609 | 9.416 | -16.620 | 9.784 | 1.00 | 43.27 |
| ATOM | 1174 | C | ARG | 1609 | 11.329 | -9.569 | 9.124 | 1.00 | 25.55 |
| ATOM | 1175 | O | ARG | 1609 | 10.469 | -9.621 | 8.231 | 1.00 | 26.98 |
| ATOM | 1176 | N | GLY | 1610 | 11.418 | -8.565 | 9.996 | 1.00 | 23.92 |
| ATOM | 1178 | CA | GLY | 1610 | 10.555 | -7.406 | 9.870 | 1.00 | 22.19 |
| ATOM | 1179 | C | GLY | 1610 | 10.800 | -6.747 | 8.512 | 1.00 | 25.92 |
| ATOM | 1180 | O | GLY | 1610 | 9.855 | -6.424 | 7.772 | 1.00 | 23.49 |
| ATOM | 1181 | N | MET | 1611 | 12.076 | -6.589 | 8.163 | 1.00 | 23.15 |
| ATOM | 1183 | CA | MET | 1611 | 12.456 | -5.989 | 6.888 | 1.00 | 22.57 |
| ATOM | 1184 | CB | MET | 1611 | 13.956 | -5.710 | 6.849 | 1.00 | 22.18 |
| ATOM | 1185 | CG | MET | 1611 | 14.398 | -4.542 | 7.729 | 1.00 | 22.63 |
| ATOM | 1186 | SD | MET | 1611 | 13.478 | -3.006 | 7.426 | 1.00 | 25.23 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1187 | CE | MET | 1611 | 13.812 | -2.688 | 5.675 | 1.00 | 21.38 |
| ATOM | 1188 | C | MET | 1611 | 12.050 | -6.848 | 5.681 | 1.00 | 23.96 |
| ATOM | 1189 | O | MET | 1611 | 11.673 | -6.326 | 4.633 | 1.00 | 25.26 |
| ATOM | 1190 | N | GLU | 1612 | 12.130 | -8.163 | 5.822 | 1.00 | 24.34 |
| ATOM | 1192 | CA | GLU | 1612 | 11.755 | -9.043 | 4.733 | 1.00 | 25.56 |
| ATOM | 1193 | CB | GLU | 1612 | 12.018 | -10.494 | 5.121 | 1.00 | 24.96 |
| ATOM | 1194 | CG | GLU | 1612 | 11.703 | -11.488 | 4.009 | 1.00 | 26.79 |
| ATOM | 1195 | CD | GLU | 1612 | 11.812 | -12.931 | 4.450 | 1.00 | 26.96 |
| ATOM | 1196 | OE1 | GLU | 1612 | 11.557 | -13.212 | 5.636 | 1.00 | 30.98 |
| ATOM | 1197 | OE2 | GLU | 1612 | 12.154 | -13.791 | 3.611 | 1.00 | 32.31 |
| ATOM | 1198 | C | GLU | 1612 | 10.267 | -8.829 | 4.415 | 1.00 | 25.70 |
| ATOM | 1199 | O | GLU | 1612 | 9.860 | -8.753 | 3.252 | 1.00 | 24.30 |
| ATOM | 1200 | N | TYR | 1613 | 9.463 | -8.723 | 5.465 | 1.00 | 23.55 |
| ATOM | 1202 | CA | TYR | 1613 | 8.037 | -8.501 | 5.294 | 1.00 | 22.94 |
| ATOM | 1203 | CB | TYR | 1613 | 7.314 | -8.586 | 6.650 | 1.00 | 24.00 |
| ATOM | 1204 | CG | TYR | 1613 | 5.841 | -8.281 | 6.549 | 1.00 | 22.93 |
| ATOM | 1205 | CD1 | TYR | 1613 | 4.945 | -9.245 | 6.097 | 1.00 | 21.60 |
| ATOM | 1206 | CE1 | TYR | 1613 | 3.582 | -8.962 | 5.963 | 1.00 | 21.14 |
| ATOM | 1207 | CD2 | TYR | 1613 | 5.347 | -7.018 | 6.869 | 1.00 | 25.81 |
| ATOM | 1208 | CE2 | TYR | 1613 | 3.979 | -6.718 | 6.733 | 1.00 | 24.45 |
| ATOM | 1209 | CZ | TYR | 1613 | 3.112 | -7.697 | 6.281 | 1.00 | 23.28 |
| ATOM | 1210 | OH | TYR | 1613 | 1.775 | -7.411 | 6.126 | 1.00 | 22.95 |
| ATOM | 1212 | C | TYR | 1613 | 7.803 | -7.138 | 4.637 | 1.00 | 22.57 |
| ATOM | 1213 | O | TYR | 1613 | 7.022 | -7.024 | 3.699 | 1.00 | 24.72 |
| ATOM | 1214 | N | LEU | 1614 | 8.460 | -6.101 | 5.156 | 1.00 | 22.16 |
| ATOM | 1216 | CA | LEU | 1614 | 8.334 | -4.755 | 4.615 | 1.00 | 22.60 |
| ATOM | 1217 | CB | LEU | 1614 | 9.175 | -3.772 | 5.440 | 1.00 | 22.56 |
| ATOM | 1218 | CG | LEU | 1614 | 8.577 | -3.415 | 6.802 | 1.00 | 24.92 |
| ATOM | 1219 | CD1 | LEU | 1614 | 9.535 | -2.541 | 7.580 | 1.00 | 21.46 |
| ATOM | 1220 | CD2 | LEU | 1614 | 7.218 | -2.711 | 6.611 | 1.00 | 21.87 |
| ATOM | 1221 | C | LEU | 1614 | 8.699 | -4.683 | 3.124 | 1.00 | 23.76 |
| ATOM | 1222 | O | LEU | 1614 | 7.975 | -4.077 | 2.326 | 1.00 | 23.84 |
| ATOM | 1223 | N | ALA | 1615 | 9.809 | -5.314 | 2.744 | 1.00 | 23.48 |
| ATOM | 1225 | CA | ALA | 1615 | 10.232 | -5.340 | 1.352 | 1.00 | 22.70 |
| ATOM | 1226 | CB | ALA | 1615 | 11.591 | -6.019 | 1.215 | 1.00 | 21.52 |
| ATOM | 1227 | C | ALA | 1615 | 9.188 | -6.063 | 0.505 | 1.00 | 22.87 |
| ATOM | 1228 | O | ALA | 1615 | 8.854 | -5.591 | -0.581 | 1.00 | 24.23 |
| ATOM | 1229 | N | SER | 1616 | 8.652 | -7.176 | 1.015 | 1.00 | 22.76 |
| ATOM | 1231 | CA | SER | 1616 | 7.638 | -7.954 | 0.295 | 1.00 | 22.88 |
| ATOM | 1232 | CB | SER | 1616 | 7.315 | -9.251 | 1.039 | 1.00 | 21.39 |
| ATOM | 1233 | OG | SER | 1616 | 6.400 | -9.036 | 2.102 | 1.00 | 26.24 |
| ATOM | 1235 | C | SER | 1616 | 6.360 | -7.131 | 0.044 | 1.00 | 24.88 |
| ATOM | 1236 | O | SER | 1616 | 5.635 | -7.358 | -0.927 | 1.00 | 24.73 |
| ATOM | 1237 | N | LYS | 1617 | 6.104 | -6.173 | 0.927 | 1.00 | 23.82 |
| ATOM | 1239 | CA | LYS | 1617 | 4.970 | -5.287 | 0.810 | 1.00 | 22.47 |
| ATOM | 1240 | CB | LYS | 1617 | 4.455 | -4.914 | 2.199 | 1.00 | 23.62 |
| ATOM | 1241 | CG | LYS | 1617 | 3.792 | -6.072 | 2.927 | 1.00 | 27.16 |
| ATOM | 1242 | CD | LYS | 1617 | 2.551 | -6.487 | 2.169 | 1.00 | 30.84 |
| ATOM | 1243 | CE | LYS | 1617 | 1.810 | -7.602 | 2.852 | 1.00 | 33.57 |
| ATOM | 1244 | NZ | LYS | 1617 | 2.484 | -8.894 | 2.653 | 1.00 | 44.30 |
| ATOM | 1248 | C | LYS | 1617 | 5.346 | -4.034 | 0.035 | 1.00 | 23.56 |
| ATOM | 1249 | O | LYS | 1617 | 4.639 | -3.030 | 0.091 | 1.00 | 25.16 |
| ATOM | 1250 | N | LYS | 1618 | 6.495 | -4.066 | -0.638 | 1.00 | 24.69 |
| ATOM | 1252 | CA | LYS | 1618 | 6.953 | -2.943 | -1.468 | 1.00 | 24.04 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1253 | CB | LYS | 1618 | 5.863 | -2.581 | -2.492 | 1.00 | 26.96 |
| ATOM | 1254 | CG | LYS | 1618 | 5.775 | -3.491 | -3.709 | 1.00 | 29.14 |
| ATOM | 1255 | CD | LYS | 1618 | 5.567 | -4.942 | -3.345 | 1.00 | 33.91 |
| ATOM | 1256 | CE | LYS | 1618 | 5.662 | -5.858 | -4.558 | 1.00 | 32.98 |
| ATOM | 1257 | NZ | LYS | 1618 | 4.431 | -5.821 | -5.380 | 1.00 | 36.73 |
| ATOM | 1261 | C | LYS | 1618 | 7.406 | -1.686 | -0.713 | 1.00 | 24.01 |
| ATOM | 1262 | O | LYS | 1618 | 7.557 | -0.606 | -1.302 | 1.00 | 23.73 |
| ATOM | 1263 | N | CYS | 1619 | 7.689 | -1.842 | 0.573 | 1.00 | 25.91 |
| ATOM | 1265 | CA | CYS | 1619 | 8.108 | -0.731 | 1.418 | 1.00 | 25.65 |
| ATOM | 1266 | CB | CYS | 1619 | 7.444 | -0.885 | 2.792 | 1.00 | 24.93 |
| ATOM | 1267 | SG | CYS | 1619 | 7.941 | 0.313 | 4.064 | 1.00 | 28.14 |
| ATOM | 1268 | C | CYS | 1619 | 9.631 | -0.628 | 1.573 | 1.00 | 23.07 |
| ATOM | 1269 | O | CYS | 1619 | 10.304 | -1.630 | 1.809 | 1.00 | 20.98 |
| ATOM | 1270 | N | ILE | 1620 | 10.170 | 0.573 | 1.363 | 1.00 | 22.95 |
| ATOM | 1272 | CA | ILE | 1620 | 11.604 | 0.841 | 1.524 | 1.00 | 23.81 |
| ATOM | 1273 | CB | ILE | 1620 | 12.202 | 1.607 | 0.276 | 1.00 | 24.36 |
| ATOM | 1274 | CG2 | ILE | 1620 | 13.670 | 1.995 | 0.506 | 1.00 | 17.24 |
| ATOM | 1275 | CG1 | ILE | 1620 | 12.108 | 0.739 | -0.987 | 1.00 | 23.13 |
| ATOM | 1276 | CD1 | ILE | 1620 | 12.171 | 1.544 | -2.286 | 1.00 | 25.37 |
| ATOM | 1277 | C | ILE | 1620 | 11.633 | 1.729 | 2.771 | 1.00 | 24.70 |
| ATOM | 1278 | O | ILE | 1620 | 10.981 | 2.763 | 2.806 | 1.00 | 25.21 |
| ATOM | 1279 | N | HIS | 1621 | 12.348 | 1.297 | 3.804 | 1.00 | 25.62 |
| ATOM | 1281 | CA | HIS | 1621 | 12.427 | 2.041 | 5.057 | 1.00 | 25.53 |
| ATOM | 1282 | CB | HIS | 1621 | 13.181 | 1.237 | 6.132 | 1.00 | 22.76 |
| ATOM | 1283 | CG | HIS | 1621 | 13.004 | 1.773 | 7.528 | 1.00 | 26.42 |
| ATOM | 1284 | CD2 | HIS | 1621 | 12.356 | 1.260 | 8.601 | 1.00 | 24.74 |
| ATOM | 1285 | ND1 | HIS | 1621 | 13.474 | 3.011 | 7.927 | 1.00 | 26.62 |
| ATOM | 1287 | CE1 | HIS | 1621 | 13.119 | 3.233 | 9.179 | 1.00 | 25.70 |
| ATOM | 1288 | NE2 | HIS | 1621 | 12.439 | 2.187 | 9.616 | 1.00 | 26.23 |
| ATOM | 1290 | C | HIS | 1621 | 13.073 | 3.401 | 4.914 | 1.00 | 26.36 |
| ATOM | 1291 | O | HIS | 1621 | 12.528 | 4.405 | 5.370 | 1.00 | 25.89 |
| ATOM | 1292 | N | ARG | 1622 | 14.271 | 3.406 | 4.341 | 1.00 | 25.35 |
| ATOM | 1294 | CA | ARG | 1622 | 15.082 | 4.608 | 4.140 | 1.00 | 25.05 |
| ATOM | 1295 | CB | ARG | 1622 | 14.268 | 5.766 | 3.540 | 1.00 | 20.89 |
| ATOM | 1296 | CG | ARG | 1622 | 13.709 | 5.444 | 2.175 | 1.00 | 19.03 |
| ATOM | 1297 | CD | ARG | 1622 | 13.089 | 6.656 | 1.488 | 0.50 | 14.06 |
| ATOM | 1298 | NE | ARG | 1622 | 12.684 | 6.300 | 0.131 | 0.50 | 11.96 |
| ATOM | 1300 | CZ | ARG | 1622 | 11.606 | 5.577 | -0.166 | 0.50 | 11.83 |
| ATOM | 1301 | NH1 | ARG | 1622 | 10.801 | 5.137 | 0.797 | 0.50 | 10.20 |
| ATOM | 1304 | NH2 | ARG | 1622 | 11.366 | 5.239 | -1.425 | 0.50 | 8.63 |
| ATOM | 1307 | C | ARG | 1622 | 15.877 | 5.058 | 5.379 | 1.00 | 24.37 |
| ATOM | 1308 | O | ARG | 1622 | 16.787 | 5.863 | 5.268 | 1.00 | 25.17 |
| ATOM | 1309 | N | ASP | 1623 | 15.555 | 4.527 | 6.552 | 1.00 | 24.61 |
| ATOM | 1311 | CA | ASP | 1623 | 16.315 | 4.899 | 7.748 | 1.00 | 28.82 |
| ATOM | 1312 | CB | ASP | 1623 | 15.777 | 6.173 | 8.410 | 1.00 | 32.33 |
| ATOM | 1313 | CG | ASP | 1623 | 16.733 | 6.735 | 9.469 | 1.00 | 36.67 |
| ATOM | 1314 | OD1 | ASP | 1623 | 16.276 | 7.520 | 10.321 | 1.00 | 43.56 |
| ATOM | 1315 | OD2 | ASP | 1623 | 17.937 | 6.385 | 9.463 | 1.00 | 36.29 |
| ATOM | 1316 | C | ASP | 1623 | 16.408 | 3.766 | 8.766 | 1.00 | 28.22 |
| ATOM | 1317 | O | ASP | 1623 | 16.118 | 3.937 | 9.956 | 1.00 | 26.87 |
| ATOM | 1318 | N | LEU | 1624 | 16.783 | 2.592 | 8.278 | 1.00 | 26.34 |
| ATOM | 1320 | CA | LEU | 1624 | 16.941 | 1.428 | 9.132 | 1.00 | 26.59 |
| ATOM | 1321 | CB | LEU | 1624 | 16.996 | 0.168 | 8.265 | 1.00 | 24.59 |
| ATOM | 1322 | CG | LEU | 1624 | 17.082 | -1.175 | 8.978 | 1.00 | 24.72 |

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ATOM   1323   CD1   LEU   1624     15.844    -1.408     9.856   1.00    24.35
ATOM   1324   CD2   LEU   1624     17.258    -2.261     7.931   1.00    24.63
ATOM   1325   C     LEU   1624     18.210     1.595    10.004   1.00    26.87
ATOM   1326   O     LEU   1624     19.322     1.777     9.497   1.00    28.19
ATOM   1327   N     ALA   1625     18.009     1.570    11.317   1.00    27.77
ATOM   1329   CA    ALA   1625     19.069     1.741    12.309   1.00    24.54
ATOM   1330   CB    ALA   1625     19.355     3.210    12.494   1.00    19.81
ATOM   1331   C     ALA   1625     18.498     1.173    13.592   1.00    26.44
ATOM   1332   O     ALA   1625     17.289     0.961    13.679   1.00    27.58
ATOM   1333   N     ALA   1626     19.342     0.940    14.594   1.00    25.38
ATOM   1335   CA    ALA   1626     18.872     0.397    15.865   1.00    24.65
ATOM   1336   CB    ALA   1626     20.054     0.023    16.774   1.00    23.35
ATOM   1337   C     ALA   1626     17.929     1.373    16.578   1.00    25.54
ATOM   1338   O     ALA   1626     17.057     0.951    17.325   1.00    27.70
ATOM   1339   N     ARG   1627     18.104     2.671    16.344   1.00    25.06
ATOM   1341   CA    ARG   1627     17.242     3.675    16.959   1.00    25.48
ATOM   1342   CB    ARG   1627     17.706     5.089    16.597   1.00    28.15
ATOM   1343   CG    ARG   1627     17.759     5.370    15.084   1.00    33.13
ATOM   1344   CD    ARG   1627     18.157     6.811    14.774   1.00    33.29
ATOM   1345   NE    ARG   1627     18.442     7.011    13.351   1.00    35.74
ATOM   1347   CZ    ARG   1627     19.652     6.889    12.813   1.00    37.40
ATOM   1348   NH1   ARG   1627     20.695     6.585    13.575   1.00    39.73
ATOM   1351   NH2   ARG   1627     19.817     7.012    11.507   1.00    36.90
ATOM   1354   C     ARG   1627     15.812     3.491    16.479   1.00    24.81
ATOM   1355   O     ARG   1627     14.871     3.853    17.173   1.00    24.05
ATOM   1356   N     ASN   1628     15.667     2.910    15.293   1.00    24.80
ATOM   1358   CA    ASN   1628     14.368     2.686    14.685   1.00    25.97
ATOM   1359   CB    ASN   1628     14.383     3.132    13.225   1.00    30.08
ATOM   1360   CG    ASN   1628     14.417     4.640    13.096   1.00    33.62
ATOM   1361   OD1   ASN   1628     13.775     5.347    13.864   1.00    35.11
ATOM   1362   ND2   ASN   1628     15.212     5.141    12.169   1.00    36.31
ATOM   1365   C     ASN   1628     13.802     1.288    14.824   1.00    26.03
ATOM   1366   O     ASN   1628     12.951     0.869    14.031   1.00    26.87
ATOM   1367   N     VAL   1629     14.330     0.550    15.797   1.00    26.04
ATOM   1369   CA    VAL   1629     13.854    -0.783    16.128   1.00    25.09
ATOM   1370   CB    VAL   1629     14.924    -1.876    15.959   1.00    27.00
ATOM   1371   CG1   VAL   1629     14.390    -3.197    16.546   1.00    20.99
ATOM   1372   CG2   VAL   1629     15.295    -2.051    14.462   1.00    23.26
ATOM   1373   C     VAL   1629     13.504    -0.671    17.600   1.00    27.59
ATOM   1374   O     VAL   1629     14.340    -0.285    18.418   1.00    25.81
ATOM   1375   N     LEU   1630     12.245    -0.929    17.923   1.00    28.17
ATOM   1377   CA    LEU   1630     11.768    -0.845    19.296   1.00    30.20
ATOM   1378   CB    LEU   1630     10.445    -0.077    19.332   1.00    30.26
ATOM   1379   CG    LEU   1630     10.484     1.285    18.626   1.00    29.81
ATOM   1380   CD1   LEU   1630      9.119     1.983    18.745   1.00    28.46
ATOM   1381   CD2   LEU   1630     11.576     2.141    19.233   1.00    28.37
ATOM   1382   C     LEU   1630     11.639    -2.242    19.904   1.00    29.32
ATOM   1383   O     LEU   1630     11.414    -3.219    19.189   1.00    30.84
ATOM   1384   N     VAL   1631     11.800    -2.342    21.221   1.00    28.90
ATOM   1386   CA    VAL   1631     11.732    -3.629    21.905   1.00    26.84
ATOM   1387   CB    VAL   1631     13.067    -3.919    22.670   1.00    28.88
ATOM   1388   CG1   VAL   1631     13.077    -5.341    23.236   1.00    21.54
ATOM   1389   CG2   VAL   1631     14.259    -3.699    21.744   1.00    24.30
ATOM   1390   C     VAL   1631     10.561    -3.645    22.881   1.00    29.02
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1391 | O | VAL | 1631 | 10.406 | -2.737 | 23.706 | 1.00 | 29.31 |
| ATOM | 1392 | N | THR | 1632 | 9.733 | -4.674 | 22.764 | 1.00 | 30.84 |
| ATOM | 1394 | CA | THR | 1632 | 8.562 | -4.830 | 23.616 | 1.00 | 32.24 |
| ATOM | 1395 | CB | THR | 1632 | 7.488 | -5.685 | 22.912 | 1.00 | 31.45 |
| ATOM | 1396 | OG1 | THR | 1632 | 7.896 | -7.064 | 22.910 | 1.00 | 30.86 |
| ATOM | 1398 | CG2 | THR | 1632 | 7.268 | -5.194 | 21.470 | 1.00 | 28.04 |
| ATOM | 1399 | C | THR | 1632 | 8.919 | -5.493 | 24.943 | 1.00 | 34.17 |
| ATOM | 1400 | O | THR | 1632 | 10.017 | -6.019 | 25.105 | 1.00 | 35.02 |
| ATOM | 1401 | N | GLU | 1633 | 7.959 | -5.524 | 25.866 | 1.00 | 36.16 |
| ATOM | 1403 | CA | GLU | 1633 | 8.155 | -6.138 | 27.177 | 1.00 | 36.34 |
| ATOM | 1404 | CB | GLU | 1633 | 6.865 | -6.063 | 27.996 | 1.00 | 37.07 |
| ATOM | 1405 | CG | GLU | 1633 | 6.957 | -6.649 | 29.414 | 1.00 | 44.57 |
| ATOM | 1406 | CD | GLU | 1633 | 8.035 | -6.000 | 30.301 | 1.00 | 49.38 |
| ATOM | 1407 | OE1 | GLU | 1633 | 8.124 | -4.753 | 30.352 | 1.00 | 51.03 |
| ATOM | 1408 | OE2 | GLU | 1633 | 8.788 | -6.750 | 30.968 | 1.00 | 51.63 |
| ATOM | 1409 | C | GLU | 1633 | 8.600 | -7.585 | 27.042 | 1.00 | 36.42 |
| ATOM | 1410 | O | GLU | 1633 | 9.347 | -8.085 | 27.874 | 1.00 | 38.56 |
| ATOM | 1411 | N | ASP | 1634 | 8.185 | -8.240 | 25.964 | 1.00 | 37.70 |
| ATOM | 1413 | CA | ASP | 1634 | 8.550 | -9.637 | 25.737 | 1.00 | 38.53 |
| ATOM | 1414 | CB | ASP | 1634 | 7.408 | -10.378 | 25.027 | 1.00 | 44.08 |
| ATOM | 1415 | CG | ASP | 1634 | 6.041 | -10.106 | 25.657 | 1.00 | 51.60 |
| ATOM | 1416 | OD1 | ASP | 1634 | 5.865 | -10.367 | 26.867 | 1.00 | 52.37 |
| ATOM | 1417 | OD2 | ASP | 1634 | 5.137 | -9.631 | 24.933 | 1.00 | 57.23 |
| ATOM | 1418 | C | ASP | 1634 | 9.826 | -9.776 | 24.905 | 1.00 | 36.56 |
| ATOM | 1419 | O | ASP | 1634 | 10.127 | -10.865 | 24.430 | 1.00 | 36.74 |
| ATOM | 1420 | N | ASN | 1635 | 10.569 | -8.683 | 24.739 | 1.00 | 36.56 |
| ATOM | 1422 | CA | ASN | 1635 | 11.819 | -8.662 | 23.945 | 1.00 | 37.10 |
| ATOM | 1423 | CB | ASN | 1635 | 12.888 | -9.587 | 24.548 | 1.00 | 36.92 |
| ATOM | 1424 | CG | ASN | 1635 | 13.226 | -9.226 | 25.978 | 1.00 | 36.54 |
| ATOM | 1425 | OD1 | ASN | 1635 | 13.275 | -8.058 | 26.340 | 1.00 | 38.84 |
| ATOM | 1426 | ND2 | ASN | 1635 | 13.423 | -10.235 | 26.806 | 1.00 | 39.58 |
| ATOM | 1429 | C | ASN | 1635 | 11.632 | -8.980 | 22.451 | 1.00 | 34.78 |
| ATOM | 1430 | O | ASN | 1635 | 12.446 | -9.677 | 21.834 | 1.00 | 34.00 |
| ATOM | 1431 | N | VAL | 1636 | 10.533 | -8.498 | 21.880 | 1.00 | 31.35 |
| ATOM | 1433 | CA | VAL | 1636 | 10.279 | -8.711 | 20.469 | 1.00 | 29.76 |
| ATOM | 1434 | CB | VAL | 1636 | 8.778 | -8.946 | 20.181 | 1.00 | 30.60 |
| ATOM | 1435 | CG1 | VAL | 1636 | 8.538 | -9.081 | 18.675 | 1.00 | 30.38 |
| ATOM | 1436 | CG2 | VAL | 1636 | 8.315 | -10.209 | 20.897 | 1.00 | 28.51 |
| ATOM | 1437 | C | VAL | 1636 | 10.768 | -7.449 | 19.781 | 1.00 | 28.02 |
| ATOM | 1438 | O | VAL | 1636 | 10.506 | -6.351 | 20.254 | 1.00 | 25.87 |
| ATOM | 1439 | N | MET | 1637 | 11.575 | -7.624 | 18.738 | 1.00 | 28.15 |
| ATOM | 1441 | CA | MET | 1637 | 12.119 | -6.508 | 17.980 | 1.00 | 26.01 |
| ATOM | 1442 | CB | MET | 1637 | 13.366 | -6.953 | 17.204 | 1.00 | 27.82 |
| ATOM | 1443 | CG | MET | 1637 | 14.479 | -7.554 | 18.051 | 1.00 | 29.73 |
| ATOM | 1444 | SD | MET | 1637 | 15.124 | -6.410 | 19.288 | 1.00 | 29.96 |
| ATOM | 1445 | CE | MET | 1637 | 15.120 | -7.459 | 20.689 | 1.00 | 27.19 |
| ATOM | 1446 | C | MET | 1637 | 11.040 | -6.087 | 16.993 | 1.00 | 24.77 |
| ATOM | 1447 | O | MET | 1637 | 10.480 | -6.929 | 16.303 | 1.00 | 24.50 |
| ATOM | 1448 | N | LYS | 1638 | 10.755 | -4.791 | 16.931 | 1.00 | 25.74 |
| ATOM | 1450 | CA | LYS | 1638 | 9.746 | -4.258 | 16.029 | 1.00 | 23.67 |
| ATOM | 1451 | CB | LYS | 1638 | 8.486 | -3.888 | 16.799 | 1.00 | 21.78 |
| ATOM | 1452 | CG | LYS | 1638 | 7.715 | -5.092 | 17.298 | 1.00 | 24.60 |
| ATOM | 1453 | CD | LYS | 1638 | 6.406 | -4.683 | 18.005 | 1.00 | 23.87 |
| ATOM | 1454 | CE | LYS | 1638 | 5.486 | -5.897 | 18.256 | 1.00 | 23.06 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1455 | NZ | LYS | 1638 | 4.871 | -6.398 | 16.976 | 1.00 | 24.60 |
| ATOM | 1459 | C | LYS | 1638 | 10.260 | -3.042 | 15.293 | 1.00 | 24.37 |
| ATOM | 1460 | O | LYS | 1638 | 10.658 | -2.055 | 15.901 | 1.00 | 26.58 |
| ATOM | 1461 | N | ILE | 1639 | 10.271 | -3.119 | 13.971 | 1.00 | 25.69 |
| ATOM | 1463 | CA | ILE | 1639 | 10.721 | -2.005 | 13.148 | 1.00 | 25.94 |
| ATOM | 1464 | CB | ILE | 1639 | 10.935 | -2.447 | 11.668 | 1.00 | 26.49 |
| ATOM | 1465 | CG2 | ILE | 1639 | 11.218 | -1.236 | 10.762 | 1.00 | 21.19 |
| ATOM | 1466 | CG1 | ILE | 1639 | 12.103 | -3.433 | 11.604 | 1.00 | 27.58 |
| ATOM | 1467 | CD1 | ILE | 1639 | 12.120 | -4.232 | 10.355 | 1.00 | 32.96 |
| ATOM | 1468 | C | ILE | 1639 | 9.675 | -0.892 | 13.242 | 1.00 | 27.32 |
| ATOM | 1469 | O | ILE | 1639 | 8.466 | -1.133 | 13.103 | 1.00 | 25.45 |
| ATOM | 1470 | N | ALA | 1640 | 10.156 | 0.320 | 13.498 | 1.00 | 27.43 |
| ATOM | 1472 | CA | ALA | 1640 | 9.321 | 1.499 | 13.632 | 1.00 | 26.96 |
| ATOM | 1473 | CB | ALA | 1640 | 9.557 | 2.133 | 15.006 | 1.00 | 25.21 |
| ATOM | 1474 | C | ALA | 1640 | 9.641 | 2.510 | 12.538 | 1.00 | 26.80 |
| ATOM | 1475 | O | ALA | 1640 | 10.691 | 2.446 | 11.896 | 1.00 | 27.55 |
| ATOM | 1476 | N | ASP | 1641 | 8.716 | 3.440 | 12.328 | 1.00 | 27.06 |
| ATOM | 1478 | CA | ASP | 1641 | 8.862 | 4.526 | 11.349 | 1.00 | 30.54 |
| ATOM | 1479 | CB | ASP | 1641 | 9.993 | 5.484 | 11.753 | 1.00 | 33.12 |
| ATOM | 1480 | CG | ASP | 1641 | 9.668 | 6.310 | 12.999 | 1.00 | 36.17 |
| ATOM | 1481 | OD1 | ASP | 1641 | 10.477 | 7.203 | 13.334 | 1.00 | 42.24 |
| ATOM | 1482 | OD2 | ASP | 1641 | 8.633 | 6.076 | 13.648 | 1.00 | 33.22 |
| ATOM | 1483 | C | ASP | 1641 | 9.049 | 4.107 | 9.898 | 1.00 | 29.94 |
| ATOM | 1484 | O | ASP | 1641 | 9.598 | 4.861 | 9.102 | 1.00 | 30.13 |
| ATOM | 1485 | N | PHE | 1642 | 8.569 | 2.920 | 9.553 | 1.00 | 30.22 |
| ATOM | 1487 | CA | PHE | 1642 | 8.680 | 2.426 | 8.191 | 1.00 | 30.91 |
| ATOM | 1488 | CB | PHE | 1642 | 8.462 | 0.909 | 8.159 | 1.00 | 26.24 |
| ATOM | 1489 | CG | PHE | 1642 | 7.156 | 0.470 | 8.750 | 1.00 | 27.82 |
| ATOM | 1490 | CD1 | PHE | 1642 | 5.986 | 0.495 | 7.988 | 1.00 | 27.08 |
| ATOM | 1491 | CD2 | PHE | 1642 | 7.089 | 0.026 | 10.066 | 1.00 | 26.70 |
| ATOM | 1492 | CE1 | PHE | 1642 | 4.761 | 0.088 | 8.532 | 1.00 | 25.18 |
| ATOM | 1493 | CE2 | PHE | 1642 | 5.872 | -0.383 | 10.624 | 1.00 | 27.59 |
| ATOM | 1494 | CZ | PHE | 1642 | 4.705 | -0.354 | 9.855 | 1.00 | 28.05 |
| ATOM | 1495 | C | PHE | 1642 | 7.729 | 3.139 | 7.219 | 1.00 | 33.35 |
| ATOM | 1496 | O | PHE | 1642 | 7.983 | 3.165 | 6.018 | 1.00 | 36.19 |
| ATOM | 1497 | N | GLY | 1643 | 6.661 | 3.746 | 7.736 | 1.00 | 32.76 |
| ATOM | 1499 | CA | GLY | 1643 | 5.710 | 4.419 | 6.863 | 1.00 | 31.44 |
| ATOM | 1500 | C | GLY | 1643 | 5.805 | 5.927 | 6.910 | 1.00 | 32.94 |
| ATOM | 1501 | O | GLY | 1643 | 4.945 | 6.636 | 6.399 | 1.00 | 33.10 |
| ATOM | 1502 | N | LEU | 1644 | 6.872 | 6.407 | 7.525 | 1.00 | 35.45 |
| ATOM | 1504 | CA | LEU | 1644 | 7.124 | 7.828 | 7.684 | 1.00 | 39.04 |
| ATOM | 1505 | CB | LEU | 1644 | 8.387 | 8.011 | 8.514 | 1.00 | 37.80 |
| ATOM | 1506 | CG | LEU | 1644 | 8.414 | 9.120 | 9.549 | 1.00 | 42.51 |
| ATOM | 1507 | CD1 | LEU | 1644 | 7.301 | 8.887 | 10.563 | 1.00 | 44.08 |
| ATOM | 1508 | CD2 | LEU | 1644 | 9.779 | 9.127 | 10.243 | 1.00 | 44.47 |
| ATOM | 1509 | C | LEU | 1644 | 7.259 | 8.580 | 6.357 | 1.00 | 42.20 |
| ATOM | 1510 | O | LEU | 1644 | 7.895 | 8.107 | 5.414 | 1.00 | 44.14 |
| ATOM | 1511 | N | ALA | 1645 | 6.607 | 9.732 | 6.267 | 1.00 | 43.89 |
| ATOM | 1513 | CA | ALA | 1645 | 6.677 | 10.569 | 5.082 | 1.00 | 45.62 |
| ATOM | 1514 | CB | ALA | 1645 | 5.463 | 11.493 | 5.028 | 1.00 | 45.06 |
| ATOM | 1515 | C | ALA | 1645 | 7.966 | 11.388 | 5.186 | 1.00 | 45.82 |
| ATOM | 1516 | O | ALA | 1645 | 8.240 | 11.994 | 6.228 | 1.00 | 45.85 |
| ATOM | 1517 | N | ARG | 1646 | 8.766 | 11.389 | 4.129 | 1.00 | 45.16 |
| ATOM | 1519 | CA | ARG | 1646 | 10.015 | 12.140 | 4.138 | 1.00 | 47.06 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1520 | CB | ARG | 1646 | 11.126 | 11.318 | 4.794 | 1.00 | 48.00 |
| ATOM | 1521 | C | ARG | 1646 | 10.445 | 12.546 | 2.742 | 1.00 | 46.83 |
| ATOM | 1522 | O | ARG | 1646 | 10.429 | 11.729 | 1.823 | 1.00 | 45.76 |
| ATOM | 1523 | N | ASP | 1647 | 10.807 | 13.814 | 2.578 | 1.00 | 48.96 |
| ATOM | 1525 | CA | ASP | 1647 | 11.278 | 14.291 | 1.288 | 1.00 | 50.93 |
| ATOM | 1526 | CB | ASP | 1647 | 10.938 | 15.769 | 1.073 | 1.00 | 52.33 |
| ATOM | 1527 | CG | ASP | 1647 | 11.191 | 16.228 | -0.360 | 1.00 | 55.93 |
| ATOM | 1528 | OD1 | ASP | 1647 | 12.231 | 15.850 | -0.956 | 1.00 | 52.58 |
| ATOM | 1529 | OD2 | ASP | 1647 | 10.340 | 16.980 | -0.896 | 1.00 | 59.54 |
| ATOM | 1530 | C | ASP | 1647 | 12.789 | 14.104 | 1.336 | 1.00 | 50.78 |
| ATOM | 1531 | O | ASP | 1647 | 13.491 | 14.803 | 2.077 | 1.00 | 48.32 |
| ATOM | 1532 | N | ILE | 1648 | 13.274 | 13.144 | 0.556 | 1.00 | 50.84 |
| ATOM | 1534 | CA | ILE | 1648 | 14.696 | 12.833 | 0.516 | 1.00 | 52.58 |
| ATOM | 1535 | CB | ILE | 1648 | 14.984 | 11.571 | -0.324 | 1.00 | 50.85 |
| ATOM | 1536 | CG2 | ILE | 1648 | 14.204 | 10.386 | 0.241 | 1.00 | 49.34 |
| ATOM | 1537 | CG1 | ILE | 1648 | 14.638 | 11.813 | -1.801 | 1.00 | 48.22 |
| ATOM | 1538 | CD1 | ILE | 1648 | 15.233 | 10.806 | -2.754 | 1.00 | 42.86 |
| ATOM | 1539 | C | ILE | 1648 | 15.523 | 13.999 | -0.018 | 1.00 | 55.57 |
| ATOM | 1540 | O | ILE | 1648 | 16.648 | 14.222 | 0.423 | 1.00 | 57.24 |
| ATOM | 1541 | N | HIS | 1649 | 14.944 | 14.766 | -0.936 | 1.00 | 56.80 |
| ATOM | 1543 | CA | HIS | 1649 | 15.650 | 15.895 | -1.520 | 1.00 | 58.03 |
| ATOM | 1544 | CB | HIS | 1649 | 15.013 | 16.302 | -2.859 | 1.00 | 58.71 |
| ATOM | 1545 | CG | HIS | 1649 | 15.221 | 15.308 | -3.958 | 1.00 | 60.28 |
| ATOM | 1546 | CD2 | HIS | 1649 | 16.303 | 14.566 | -4.306 | 1.00 | 60.74 |
| ATOM | 1547 | ND1 | HIS | 1649 | 14.241 | 14.986 | -4.874 | 1.00 | 61.70 |
| ATOM | 1549 | CE1 | HIS | 1649 | 14.708 | 14.104 | -5.742 | 1.00 | 61.86 |
| ATOM | 1550 | NE2 | HIS | 1649 | 15.959 | 13.833 | -5.417 | 1.00 | 60.98 |
| ATOM | 1552 | C | HIS | 1649 | 15.721 | 17.093 | -0.591 | 1.00 | 58.49 |
| ATOM | 1553 | O | HIS | 1649 | 16.129 | 18.175 | -1.004 | 1.00 | 60.56 |
| ATOM | 1554 | N | HIS | 1650 | 15.285 | 16.916 | 0.654 | 1.00 | 59.58 |
| ATOM | 1556 | CA | HIS | 1650 | 15.306 | 18.001 | 1.635 | 1.00 | 61.38 |
| ATOM | 1557 | CB | HIS | 1650 | 13.898 | 18.540 | 1.863 | 1.00 | 65.28 |
| ATOM | 1558 | CG | HIS | 1650 | 13.404 | 19.433 | 0.738 | 1.00 | 72.62 |
| ATOM | 1559 | CD2 | HIS | 1650 | 13.492 | 20.752 | 0.536 | 1.00 | 76.23 |
| ATOM | 1560 | ND1 | HIS | 1650 | 12.710 | 18.904 | -0.339 | 1.00 | 77.05 |
| ATOM | 1562 | CE1 | HIS | 1650 | 12.402 | 19.907 | -1.157 | 1.00 | 78.51 |
| ATOM | 1563 | NE2 | HIS | 1650 | 12.863 | 21.015 | -0.647 | 1.00 | 78.82 |
| ATOM | 1565 | C | HIS | 1650 | 15.925 | 17.575 | 2.972 | 1.00 | 60.63 |
| ATOM | 1566 | O | HIS | 1650 | 15.796 | 18.271 | 3.969 | 1.00 | 60.20 |
| ATOM | 1567 | N | ILE | 1651 | 16.584 | 16.419 | 2.987 | 1.00 | 60.22 |
| ATOM | 1569 | CA | ILE | 1651 | 17.197 | 15.920 | 4.204 | 1.00 | 60.03 |
| ATOM | 1570 | CB | ILE | 1651 | 17.574 | 14.434 | 4.069 | 1.00 | 62.54 |
| ATOM | 1571 | CG2 | ILE | 1651 | 18.280 | 13.920 | 5.323 | 1.00 | 63.48 |
| ATOM | 1572 | CG1 | ILE | 1651 | 16.329 | 13.584 | 3.800 | 1.00 | 65.18 |
| ATOM | 1573 | CD1 | ILE | 1651 | 16.635 | 12.124 | 3.603 | 1.00 | 67.18 |
| ATOM | 1574 | C | ILE | 1651 | 18.457 | 16.698 | 4.557 | 1.00 | 59.16 |
| ATOM | 1575 | O | ILE | 1651 | 19.326 | 16.907 | 3.716 | 1.00 | 59.25 |
| ATOM | 1576 | N | ASP | 1652 | 18.532 | 17.176 | 5.793 | 1.00 | 58.91 |
| ATOM | 1578 | CA | ASP | 1652 | 19.702 | 17.915 | 6.260 | 1.00 | 58.25 |
| ATOM | 1579 | CB | ASP | 1652 | 19.312 | 18.788 | 7.444 | 1.00 | 61.14 |
| ATOM | 1580 | CG | ASP | 1652 | 20.506 | 19.569 | 8.028 | 1.00 | 65.33 |
| ATOM | 1581 | OD1 | ASP | 1652 | 21.614 | 19.574 | 7.411 | 1.00 | 67.11 |
| ATOM | 1582 | OD2 | ASP | 1652 | 20.337 | 20.191 | 9.126 | 1.00 | 69.04 |
| ATOM | 1583 | C | ASP | 1652 | 20.786 | 16.922 | 6.676 | 1.00 | 56.75 |

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ATOM   1584  O    ASP  1652    20.699   16.307    7.741   1.00   56.06
ATOM   1585  N    TYR  1653    21.794   16.762    5.826   1.00   55.40
ATOM   1587  CA   TYR  1653    22.900   15.849    6.088   1.00   54.50
ATOM   1588  CB   TYR  1653    23.825   15.783    4.872   1.00   52.80
ATOM   1589  CG   TYR  1653    23.334   14.854    3.796   1.00   52.10
ATOM   1590  CD1  TYR  1653    24.123   14.566    2.685   1.00   51.50
ATOM   1591  CE1  TYR  1653    23.701   13.658    1.724   1.00   53.52
ATOM   1592  CD2  TYR  1653    22.099   14.214    3.917   1.00   52.88
ATOM   1593  CE2  TYR  1653    21.664   13.302    2.966   1.00   54.63
ATOM   1594  CZ   TYR  1653    22.469   13.025    1.870   1.00   54.35
ATOM   1595  OH   TYR  1653    22.049   12.107    0.933   1.00   53.23
ATOM   1597  C    TYR  1653    23.717   16.158    7.339   1.00   55.40
ATOM   1598  O    TYR  1653    24.381   15.284    7.900   1.00   54.47
ATOM   1599  N    TYR  1654    23.673   17.409    7.773   1.00   56.72
ATOM   1601  CA   TYR  1654    24.421   17.826    8.947   1.00   58.87
ATOM   1602  CB   TYR  1654    24.978   19.235    8.733   1.00   57.91
ATOM   1603  CG   TYR  1654    26.068   19.269    7.685   1.00   60.49
ATOM   1604  CD1  TYR  1654    25.760   19.301    6.325   1.00   61.37
ATOM   1605  CE1  TYR  1654    26.769   19.289    5.356   1.00   63.72
ATOM   1606  CD2  TYR  1654    27.412   19.227    8.053   1.00   61.74
ATOM   1607  CE2  TYR  1654    28.425   19.216    7.099   1.00   64.08
ATOM   1608  CZ   TYR  1654    28.102   19.248    5.753   1.00   65.12
ATOM   1609  OH   TYR  1654    29.117   19.248    4.817   1.00   64.17
ATOM   1611  C    TYR  1654    23.628   17.732   10.245   1.00   60.17
ATOM   1612  O    TYR  1654    24.173   17.935   11.335   1.00   61.09
ATOM   1613  N    LYS  1655    22.348   17.393   10.133   1.00   60.54
ATOM   1615  CA   LYS  1655    21.493   17.277   11.306   1.00   62.12
ATOM   1616  CB   LYS  1655    20.019   17.382   10.910   1.00   64.32
ATOM   1617  CG   LYS  1655    19.054   17.346   12.079   1.00   67.17
ATOM   1618  CD   LYS  1655    17.644   17.608   11.602   1.00   73.05
ATOM   1619  CE   LYS  1655    16.626   17.243   12.660   1.00   77.36
ATOM   1620  NZ   LYS  1655    15.230   17.494   12.186   1.00   81.10
ATOM   1624  C    LYS  1655    21.754   15.976   12.057   1.00   62.19
ATOM   1625  O    LYS  1655    21.902   14.907   11.454   1.00   61.36
ATOM   1626  N    LYS  1656    21.822   16.084   13.380   1.00   62.26
ATOM   1628  CA   LYS  1656    22.069   14.933   14.236   1.00   62.28
ATOM   1629  CB   LYS  1656    23.027   15.310   15.372   1.00   62.05
ATOM   1630  CG   LYS  1656    24.474   15.489   14.957   1.00   62.62
ATOM   1631  CD   LYS  1656    25.320   15.889   16.157   1.00   66.45
ATOM   1632  CE   LYS  1656    26.803   15.666   15.908   1.00   67.28
ATOM   1633  NZ   LYS  1656    27.619   16.007   17.109   1.00   68.45
ATOM   1637  C    LYS  1656    20.774   14.381   14.824   1.00   61.86
ATOM   1638  O    LYS  1656    19.714   15.007   14.733   1.00   62.95
ATOM   1639  N    THR  1657    20.875   13.198   15.420   1.00   60.10
ATOM   1641  CA   THR  1657    19.743   12.541   16.053   1.00   57.73
ATOM   1642  CB   THR  1657    19.973   11.012   16.121   1.00   56.04
ATOM   1643  OG1  THR  1657    21.150   10.730   16.896   1.00   55.21
ATOM   1645  CG2  THR  1657    20.152   10.431   14.731   1.00   53.07
ATOM   1646  C    THR  1657    19.664   13.102   17.472   1.00   57.74
ATOM   1647  O    THR  1657    20.513   13.899   17.870   1.00   57.76
ATOM   1648  N    THR  1658    18.678   12.667   18.249   1.00   58.80
ATOM   1650  CA   THR  1658    18.548   13.140   19.627   1.00   60.33
ATOM   1651  CB   THR  1658    17.318   12.517   20.290   1.00   61.37
ATOM   1652  C    THR  1658    19.811   12.779   20.406   1.00   60.43
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1653 | O | THR | 1658 | 20.350 | 13.599 | 21.155 | 1.00 | 60.59 |
| ATOM | 1654 | N | ASN | 1659 | 20.311 | 11.567 | 20.161 | 1.00 | 59.97 |
| ATOM | 1656 | CA | ASN | 1659 | 21.508 | 11.058 | 20.827 | 1.00 | 58.28 |
| ATOM | 1657 | CB | ASN | 1659 | 21.607 | 9.545 | 20.645 | 1.00 | 59.95 |
| ATOM | 1658 | CG | ASN | 1659 | 22.444 | 8.883 | 21.723 | 1.00 | 60.10 |
| ATOM | 1659 | OD1 | ASN | 1659 | 22.382 | 9.265 | 22.891 | 1.00 | 61.26 |
| ATOM | 1660 | ND2 | ASN | 1659 | 23.210 | 7.867 | 21.341 | 1.00 | 57.09 |
| ATOM | 1663 | C | ASN | 1659 | 22.781 | 11.717 | 20.311 | 1.00 | 57.13 |
| ATOM | 1664 | O | ASN | 1659 | 23.868 | 11.418 | 20.793 | 1.00 | 57.34 |
| ATOM | 1665 | N | GLY | 1660 | 22.643 | 12.570 | 19.299 | 1.00 | 56.48 |
| ATOM | 1667 | CA | GLY | 1660 | 23.781 | 13.276 | 18.733 | 1.00 | 54.87 |
| ATOM | 1668 | C | GLY | 1660 | 24.539 | 12.570 | 17.623 | 1.00 | 53.04 |
| ATOM | 1669 | O | GLY | 1660 | 25.716 | 12.855 | 17.394 | 1.00 | 54.11 |
| ATOM | 1670 | N | ARG | 1661 | 23.879 | 11.659 | 16.918 | 1.00 | 51.37 |
| ATOM | 1672 | CA | ARG | 1661 | 24.536 | 10.930 | 15.833 | 1.00 | 48.96 |
| ATOM | 1673 | CB | ARG | 1661 | 24.283 | 9.428 | 15.961 | 1.00 | 48.48 |
| ATOM | 1674 | CG | ARG | 1661 | 24.848 | 8.796 | 17.215 | 1.00 | 50.03 |
| ATOM | 1675 | CD | ARG | 1661 | 24.492 | 7.325 | 17.234 | 1.00 | 50.78 |
| ATOM | 1676 | NE | ARG | 1661 | 25.013 | 6.614 | 18.396 | 1.00 | 50.11 |
| ATOM | 1678 | CZ | ARG | 1661 | 24.902 | 5.299 | 18.566 | 1.00 | 50.08 |
| ATOM | 1679 | NH1 | ARG | 1661 | 24.286 | 4.560 | 17.645 | 1.00 | 46.57 |
| ATOM | 1682 | NH2 | ARG | 1661 | 25.426 | 4.717 | 19.643 | 1.00 | 47.88 |
| ATOM | 1685 | C | ARG | 1661 | 24.076 | 11.422 | 14.459 | 1.00 | 46.53 |
| ATOM | 1686 | O | ARG | 1661 | 23.031 | 12.029 | 14.325 | 1.00 | 45.01 |
| ATOM | 1687 | N | LEU | 1662 | 24.839 | 11.094 | 13.432 | 1.00 | 42.39 |
| ATOM | 1689 | CA | LEU | 1662 | 24.546 | 11.503 | 12.076 | 1.00 | 40.71 |
| ATOM | 1690 | CB | LEU | 1662 | 25.823 | 12.031 | 11.399 | 1.00 | 40.25 |
| ATOM | 1691 | CG | LEU | 1662 | 26.408 | 13.332 | 11.965 | 1.00 | 42.44 |
| ATOM | 1692 | CD1 | LEU | 1662 | 27.853 | 13.478 | 11.537 | 1.00 | 40.42 |
| ATOM | 1693 | CD2 | LEU | 1662 | 25.591 | 14.536 | 11.514 | 1.00 | 41.16 |
| ATOM | 1694 | C | LEU | 1662 | 23.946 | 10.362 | 11.258 | 1.00 | 38.45 |
| ATOM | 1695 | O | LEU | 1662 | 24.647 | 9.436 | 10.862 | 1.00 | 36.67 |
| ATOM | 1696 | N | PRO | 1663 | 22.632 | 10.428 | 10.987 | 1.00 | 37.09 |
| ATOM | 1697 | CD | PRO | 1663 | 21.717 | 11.475 | 11.489 | 1.00 | 38.18 |
| ATOM | 1698 | CA | PRO | 1663 | 21.894 | 9.424 | 10.207 | 1.00 | 35.59 |
| ATOM | 1699 | CB | PRO | 1663 | 20.535 | 10.098 | 9.983 | 1.00 | 35.90 |
| ATOM | 1700 | CG | PRO | 1663 | 20.343 | 10.856 | 11.258 | 1.00 | 39.13 |
| ATOM | 1701 | C | PRO | 1663 | 22.556 | 9.045 | 8.876 | 1.00 | 33.05 |
| ATOM | 1702 | O | PRO | 1663 | 22.362 | 7.933 | 8.378 | 1.00 | 31.16 |
| ATOM | 1703 | N | VAL | 1664 | 23.333 | 9.960 | 8.299 | 1.00 | 32.07 |
| ATOM | 1705 | CA | VAL | 1664 | 24.020 | 9.669 | 7.034 | 1.00 | 32.49 |
| ATOM | 1706 | CB | VAL | 1664 | 24.831 | 10.886 | 6.477 | 1.00 | 32.68 |
| ATOM | 1707 | CG1 | VAL | 1664 | 23.898 | 11.906 | 5.864 | 1.00 | 32.25 |
| ATOM | 1708 | CG2 | VAL | 1664 | 25.670 | 11.523 | 7.571 | 1.00 | 33.22 |
| ATOM | 1709 | C | VAL | 1664 | 24.957 | 8.469 | 7.171 | 1.00 | 29.57 |
| ATOM | 1710 | O | VAL | 1664 | 25.328 | 7.864 | 6.175 | 1.00 | 27.39 |
| ATOM | 1711 | N | LYS | 1665 | 25.303 | 8.116 | 8.409 | 1.00 | 28.82 |
| ATOM | 1713 | CA | LYS | 1665 | 26.189 | 6.991 | 8.673 | 1.00 | 27.87 |
| ATOM | 1714 | CB | LYS | 1665 | 26.815 | 7.100 | 10.065 | 1.00 | 26.99 |
| ATOM | 1715 | CG | LYS | 1665 | 27.967 | 8.089 | 10.079 | 1.00 | 29.23 |
| ATOM | 1716 | CD | LYS | 1665 | 28.283 | 8.619 | 11.466 | 1.00 | 30.64 |
| ATOM | 1717 | CE | LYS | 1665 | 29.543 | 9.478 | 11.426 | 1.00 | 30.94 |
| ATOM | 1718 | NZ | LYS | 1665 | 29.826 | 10.128 | 12.737 | 1.00 | 31.63 |
| ATOM | 1722 | C | LYS | 1665 | 25.546 | 5.637 | 8.465 | 1.00 | 26.76 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1723 | O | LYS | 1665 | 26.211 | 4.615 | 8.589 | 1.00 | 26.78 |
| ATOM | 1724 | N | TRP | 1666 | 24.260 | 5.630 | 8.137 | 1.00 | 25.79 |
| ATOM | 1726 | CA | TRP | 1666 | 23.561 | 4.381 | 7.865 | 1.00 | 26.56 |
| ATOM | 1727 | CB | TRP | 1666 | 22.299 | 4.273 | 8.724 | 1.00 | 25.63 |
| ATOM | 1728 | CG | TRP | 1666 | 22.564 | 3.872 | 10.174 | 1.00 | 26.95 |
| ATOM | 1729 | CD2 | TRP | 1666 | 23.052 | 4.717 | 11.232 | 1.00 | 24.83 |
| ATOM | 1730 | CE2 | TRP | 1666 | 23.134 | 3.920 | 12.398 | 1.00 | 24.49 |
| ATOM | 1731 | CE3 | TRP | 1666 | 23.433 | 6.062 | 11.306 | 1.00 | 24.54 |
| ATOM | 1732 | CD1 | TRP | 1666 | 22.376 | 2.636 | 10.730 | 1.00 | 20.10 |
| ATOM | 1733 | NE1 | TRP | 1666 | 22.716 | 2.660 | 12.063 | 1.00 | 21.86 |
| ATOM | 1735 | CZ2 | TRP | 1666 | 23.575 | 4.433 | 13.627 | 1.00 | 25.71 |
| ATOM | 1736 | CZ3 | TRP | 1666 | 23.870 | 6.569 | 12.523 | 1.00 | 26.00 |
| ATOM | 1737 | CH2 | TRP | 1666 | 23.939 | 5.754 | 13.665 | 1.00 | 26.04 |
| ATOM | 1738 | C | TRP | 1666 | 23.188 | 4.263 | 6.386 | 1.00 | 23.62 |
| ATOM | 1739 | O | TRP | 1666 | 22.754 | 3.214 | 5.931 | 1.00 | 24.87 |
| ATOM | 1740 | N | MET | 1667 | 23.404 | 5.330 | 5.631 | 1.00 | 22.78 |
| ATOM | 1742 | CA | MET | 1667 | 23.046 | 5.361 | 4.215 | 1.00 | 23.73 |
| ATOM | 1743 | CB | MET | 1667 | 22.894 | 6.802 | 3.744 | 1.00 | 26.24 |
| ATOM | 1744 | CG | MET | 1667 | 21.823 | 7.621 | 4.434 | 1.00 | 35.55 |
| ATOM | 1745 | SD | MET | 1667 | 21.795 | 9.276 | 3.706 | 1.00 | 42.23 |
| ATOM | 1746 | CE | MET | 1667 | 21.019 | 8.904 | 2.238 | 1.00 | 40.57 |
| ATOM | 1747 | C | MET | 1667 | 23.991 | 4.693 | 3.239 | 1.00 | 22.77 |
| ATOM | 1748 | O | MET | 1667 | 25.205 | 4.894 | 3.294 | 1.00 | 24.25 |
| ATOM | 1749 | N | ALA | 1668 | 23.420 | 3.963 | 2.286 | 1.00 | 22.73 |
| ATOM | 1751 | CA | ALA | 1668 | 24.217 | 3.337 | 1.237 | 1.00 | 23.54 |
| ATOM | 1752 | CB | ALA | 1668 | 23.339 | 2.495 | 0.340 | 1.00 | 21.80 |
| ATOM | 1753 | C | ALA | 1668 | 24.805 | 4.495 | 0.430 | 1.00 | 25.53 |
| ATOM | 1754 | O | ALA | 1668 | 24.181 | 5.551 | 0.316 | 1.00 | 23.66 |
| ATOM | 1755 | N | PRO | 1669 | 26.006 | 4.314 | -0.153 | 1.00 | 26.86 |
| ATOM | 1756 | CD | PRO | 1669 | 26.899 | 3.144 | -0.095 | 1.00 | 26.35 |
| ATOM | 1757 | CA | PRO | 1669 | 26.611 | 5.390 | -0.942 | 1.00 | 27.78 |
| ATOM | 1758 | CB | PRO | 1669 | 27.864 | 4.731 | -1.518 | 1.00 | 25.51 |
| ATOM | 1759 | CG | PRO | 1669 | 28.225 | 3.741 | -0.471 | 1.00 | 25.36 |
| ATOM | 1760 | C | PRO | 1669 | 25.686 | 5.900 | -2.057 | 1.00 | 26.47 |
| ATOM | 1761 | O | PRO | 1669 | 25.617 | 7.099 | -2.288 | 1.00 | 28.42 |
| ATOM | 1762 | N | GLU | 1670 | 24.951 | 5.010 | -2.724 | 1.00 | 26.88 |
| ATOM | 1764 | CA | GLU | 1670 | 24.057 | 5.459 | -3.796 | 1.00 | 29.03 |
| ATOM | 1765 | CB | GLU | 1670 | 23.597 | 4.293 | -4.693 | 1.00 | 31.79 |
| ATOM | 1766 | CG | GLU | 1670 | 22.588 | 3.325 | -4.065 | 1.00 | 32.47 |
| ATOM | 1767 | CD | GLU | 1670 | 23.212 | 2.184 | -3.255 | 1.00 | 32.43 |
| ATOM | 1768 | OE1 | GLU | 1670 | 22.429 | 1.297 | -2.822 | 1.00 | 25.01 |
| ATOM | 1769 | OE2 | GLU | 1670 | 24.458 | 2.157 | -3.069 | 1.00 | 28.75 |
| ATOM | 1770 | C | GLU | 1670 | 22.864 | 6.274 | -3.294 | 1.00 | 28.37 |
| ATOM | 1771 | O | GLU | 1670 | 22.358 | 7.146 | -4.001 | 1.00 | 25.72 |
| ATOM | 1772 | N | ALA | 1671 | 22.451 | 6.028 | -2.053 | 1.00 | 30.08 |
| ATOM | 1774 | CA | ALA | 1671 | 21.347 | 6.779 | -1.465 | 1.00 | 31.24 |
| ATOM | 1775 | CB | ALA | 1671 | 20.751 | 6.031 | -0.287 | 1.00 | 26.42 |
| ATOM | 1776 | C | ALA | 1671 | 21.899 | 8.125 | -1.013 | 1.00 | 31.36 |
| ATOM | 1777 | O | ALA | 1671 | 21.298 | 9.167 | -1.249 | 1.00 | 33.11 |
| ATOM | 1778 | N | LEU | 1672 | 23.068 | 8.096 | -0.387 | 1.00 | 32.73 |
| ATOM | 1780 | CA | LEU | 1672 | 23.715 | 9.304 | 0.100 | 1.00 | 33.96 |
| ATOM | 1781 | CB | LEU | 1672 | 24.931 | 8.935 | 0.940 | 1.00 | 33.89 |
| ATOM | 1782 | CG | LEU | 1672 | 25.783 | 10.071 | 1.502 | 1.00 | 37.62 |
| ATOM | 1783 | CD1 | LEU | 1672 | 25.010 | 10.800 | 2.581 | 1.00 | 39.57 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1784 | CD2 | LEU | 1672 | 27.054 | 9.491 | 2.087 | 1.00 | 32.30 |
| ATOM | 1785 | C | LEU | 1672 | 24.157 | 10.207 | -1.042 | 1.00 | 36.83 |
| ATOM | 1786 | O | LEU | 1672 | 23.769 | 11.369 | -1.102 | 1.00 | 37.87 |
| ATOM | 1787 | N | PHE | 1673 | 24.959 | 9.669 | -1.954 | 1.00 | 35.82 |
| ATOM | 1789 | CA | PHE | 1673 | 25.466 | 10.449 | -3.071 | 1.00 | 35.82 |
| ATOM | 1790 | CB | PHE | 1673 | 26.738 | 9.802 | -3.639 | 1.00 | 34.66 |
| ATOM | 1791 | CG | PHE | 1673 | 27.850 | 9.642 | -2.634 | 1.00 | 33.84 |
| ATOM | 1792 | CD1 | PHE | 1673 | 28.503 | 8.422 | -2.494 | 1.00 | 32.65 |
| ATOM | 1793 | CD2 | PHE | 1673 | 28.242 | 10.709 | -1.827 | 1.00 | 36.98 |
| ATOM | 1794 | CE1 | PHE | 1673 | 29.540 | 8.257 | -1.555 | 1.00 | 37.95 |
| ATOM | 1795 | CE2 | PHE | 1673 | 29.279 | 10.557 | -0.881 | 1.00 | 39.90 |
| ATOM | 1796 | CZ | PHE | 1673 | 29.927 | 9.325 | -0.748 | 1.00 | 37.09 |
| ATOM | 1797 | C | PHE | 1673 | 24.483 | 10.692 | -4.210 | 1.00 | 36.34 |
| ATOM | 1798 | O | PHE | 1673 | 24.430 | 11.788 | -4.754 | 1.00 | 37.18 |
| ATOM | 1799 | N | ASP | 1674 | 23.705 | 9.677 | -4.568 | 1.00 | 38.22 |
| ATOM | 1801 | CA | ASP | 1674 | 22.780 | 9.777 | -5.693 | 1.00 | 38.51 |
| ATOM | 1802 | CB | ASP | 1674 | 23.008 | 8.597 | -6.633 | 1.00 | 40.34 |
| ATOM | 1803 | CG | ASP | 1674 | 24.439 | 8.511 | -7.122 | 1.00 | 43.87 |
| ATOM | 1804 | OD1 | ASP | 1674 | 25.092 | 9.571 | -7.254 | 1.00 | 42.79 |
| ATOM | 1805 | OD2 | ASP | 1674 | 24.906 | 7.376 | -7.369 | 1.00 | 47.94 |
| ATOM | 1806 | C | ASP | 1674 | 21.298 | 9.853 | -5.360 | 1.00 | 40.21 |
| ATOM | 1807 | O | ASP | 1674 | 20.457 | 9.872 | -6.271 | 1.00 | 39.07 |
| ATOM | 1808 | N | ARG | 1675 | 20.975 | 9.836 | -4.072 | 1.00 | 39.83 |
| ATOM | 1810 | CA | ARG | 1675 | 19.589 | 9.900 | -3.631 | 1.00 | 42.25 |
| ATOM | 1811 | CB | ARG | 1675 | 18.992 | 11.271 | -3.964 | 1.00 | 48.19 |
| ATOM | 1812 | CG | ARG | 1675 | 19.691 | 12.420 | -3.267 | 1.00 | 59.20 |
| ATOM | 1813 | CD | ARG | 1675 | 19.462 | 13.729 | -4.019 | 1.00 | 67.81 |
| ATOM | 1814 | NE | ARG | 1675 | 20.079 | 14.876 | -3.352 | 1.00 | 75.11 |
| ATOM | 1816 | CZ | ARG | 1675 | 19.688 | 16.136 | -3.525 | 1.00 | 78.74 |
| ATOM | 1817 | NH1 | ARG | 1675 | 18.680 | 16.429 | -4.341 | 1.00 | 79.91 |
| ATOM | 1820 | NH2 | ARG | 1675 | 20.311 | 17.115 | -2.890 | 1.00 | 81.24 |
| ATOM | 1823 | C | ARG | 1675 | 18.730 | 8.777 | -4.221 | 1.00 | 39.00 |
| ATOM | 1824 | O | ARG | 1675 | 17.544 | 8.956 | -4.488 | 1.00 | 39.71 |
| ATOM | 1825 | N | ILE | 1676 | 19.345 | 7.624 | -4.434 | 1.00 | 35.50 |
| ATOM | 1827 | CA | ILE | 1676 | 18.636 | 6.471 | -4.958 | 1.00 | 33.51 |
| ATOM | 1828 | CB | ILE | 1676 | 19.434 | 5.759 | -6.039 | 1.00 | 34.59 |
| ATOM | 1829 | CG2 | ILE | 1676 | 18.582 | 4.678 | -6.649 | 1.00 | 33.90 |
| ATOM | 1830 | CG1 | ILE | 1676 | 19.848 | 6.752 | -7.120 | 1.00 | 37.60 |
| ATOM | 1831 | CD1 | ILE | 1676 | 20.861 | 6.197 | -8.109 | 1.00 | 42.67 |
| ATOM | 1832 | C | ILE | 1676 | 18.390 | 5.501 | -3.809 | 1.00 | 30.94 |
| ATOM | 1833 | O | ILE | 1676 | 19.326 | 4.926 | -3.252 | 1.00 | 28.62 |
| ATOM | 1834 | N | TYR | 1677 | 17.124 | 5.351 | -3.443 | 1.00 | 30.60 |
| ATOM | 1836 | CA | TYR | 1677 | 16.724 | 4.467 | -2.359 | 1.00 | 25.87 |
| ATOM | 1837 | CB | TYR | 1677 | 15.781 | 5.197 | -1.413 | 1.00 | 26.40 |
| ATOM | 1838 | CG | TYR | 1677 | 16.483 | 6.220 | -0.555 | 1.00 | 27.67 |
| ATOM | 1839 | CD1 | TYR | 1677 | 16.663 | 7.533 | -0.999 | 1.00 | 27.45 |
| ATOM | 1840 | CE1 | TYR | 1677 | 17.269 | 8.483 | -0.191 | 1.00 | 26.55 |
| ATOM | 1841 | CD2 | TYR | 1677 | 16.935 | 5.883 | 0.721 | 1.00 | 24.58 |
| ATOM | 1842 | CE2 | TYR | 1677 | 17.536 | 6.828 | 1.538 | 1.00 | 26.35 |
| ATOM | 1843 | CZ | TYR | 1677 | 17.698 | 8.122 | 1.080 | 1.00 | 28.80 |
| ATOM | 1844 | OH | TYR | 1677 | 18.270 | 9.059 | 1.914 | 1.00 | 34.97 |
| ATOM | 1846 | C | TYR | 1677 | 16.055 | 3.235 | -2.911 | 1.00 | 22.70 |
| ATOM | 1847 | O | TYR | 1677 | 15.144 | 3.335 | -3.728 | 1.00 | 26.22 |
| ATOM | 1848 | N | THR | 1678 | 16.477 | 2.076 | -2.420 | 1.00 | 21.83 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1850 | CA | THR | 1678 | 15.968 | 0.791 | -2.865 | 1.00 | 22.14 |
| ATOM | 1851 | CB | THR | 1678 | 16.907 | 0.191 | -3.928 | 1.00 | 23.91 |
| ATOM | 1852 | OG1 | THR | 1678 | 18.229 | 0.105 | -3.373 | 1.00 | 27.47 |
| ATOM | 1854 | CG2 | THR | 1678 | 16.949 | 1.053 | -5.188 | 1.00 | 24.94 |
| ATOM | 1855 | C | THR | 1678 | 15.999 | -0.176 | -1.692 | 1.00 | 22.79 |
| ATOM | 1856 | O | THR | 1678 | 16.427 | 0.170 | -0.592 | 1.00 | 23.39 |
| ATOM | 1857 | N | HIS | 1679 | 15.563 | -1.402 | -1.929 | 1.00 | 21.98 |
| ATOM | 1859 | CA | HIS | 1679 | 15.613 | -2.417 | -0.888 | 1.00 | 22.97 |
| ATOM | 1860 | CB | HIS | 1679 | 14.872 | -3.671 | -1.351 | 1.00 | 22.04 |
| ATOM | 1861 | CG | HIS | 1679 | 13.421 | -3.444 | -1.621 | 1.00 | 25.41 |
| ATOM | 1862 | CD2 | HIS | 1679 | 12.674 | -3.611 | -2.740 | 1.00 | 26.60 |
| ATOM | 1863 | ND1 | HIS | 1679 | 12.556 | -2.954 | -0.663 | 1.00 | 26.13 |
| ATOM | 1865 | CE1 | HIS | 1679 | 11.348 | -2.830 | -1.178 | 1.00 | 28.66 |
| ATOM | 1866 | NE2 | HIS | 1679 | 11.394 | -3.221 | -2.441 | 1.00 | 29.66 |
| ATOM | 1868 | C | HIS | 1679 | 17.097 | -2.719 | -0.650 | 1.00 | 23.14 |
| ATOM | 1869 | O | HIS | 1679 | 17.511 | -3.074 | 0.459 | 1.00 | 21.69 |
| ATOM | 1870 | N | GLN | 1680 | 17.895 | -2.506 | -1.697 | 1.00 | 22.38 |
| ATOM | 1872 | CA | GLN | 1680 | 19.335 | -2.726 | -1.658 | 1.00 | 22.33 |
| ATOM | 1873 | CB | GLN | 1680 | 19.948 | -2.594 | -3.058 | 1.00 | 22.52 |
| ATOM | 1874 | CG | GLN | 1680 | 19.895 | -3.872 | -3.879 | 1.00 | 29.15 |
| ATOM | 1875 | CD | GLN | 1680 | 18.865 | -3.847 | -4.991 | 1.00 | 33.60 |
| ATOM | 1876 | OE1 | GLN | 1680 | 17.819 | -3.212 | -4.871 | 1.00 | 38.43 |
| ATOM | 1877 | NE2 | GLN | 1680 | 19.159 | -4.542 | -6.085 | 1.00 | 33.44 |
| ATOM | 1880 | C | GLN | 1680 | 20.007 | -1.740 | -0.732 | 1.00 | 22.61 |
| ATOM | 1881 | O | GLN | 1680 | 20.943 | -2.093 | -0.027 | 1.00 | 22.00 |
| ATOM | 1882 | N | SER | 1681 | 19.562 | -0.490 | -0.745 | 1.00 | 22.06 |
| ATOM | 1884 | CA | SER | 1681 | 20.184 | 0.479 | 0.137 | 1.00 | 23.41 |
| ATOM | 1885 | CB | SER | 1681 | 19.886 | 1.923 | -0.306 | 1.00 | 20.06 |
| ATOM | 1886 | OG | SER | 1681 | 18.503 | 2.166 | -0.479 | 1.00 | 22.90 |
| ATOM | 1888 | C | SER | 1681 | 19.778 | 0.206 | 1.583 | 1.00 | 23.08 |
| ATOM | 1889 | O | SER | 1681 | 20.528 | 0.531 | 2.506 | 1.00 | 24.13 |
| ATOM | 1890 | N | ASP | 1682 | 18.608 | -0.412 | 1.770 | 1.00 | 23.19 |
| ATOM | 1892 | CA | ASP | 1682 | 18.107 | -0.775 | 3.104 | 1.00 | 22.37 |
| ATOM | 1893 | CB | ASP | 1682 | 16.660 | -1.275 | 3.018 | 1.00 | 24.55 |
| ATOM | 1894 | CG | ASP | 1682 | 15.616 | -0.172 | 3.222 | 1.00 | 24.22 |
| ATOM | 1895 | OD1 | ASP | 1682 | 14.428 | -0.479 | 3.005 | 1.00 | 25.02 |
| ATOM | 1896 | OD2 | ASP | 1682 | 15.949 | 0.968 | 3.625 | 1.00 | 24.82 |
| ATOM | 1897 | C | ASP | 1682 | 18.980 | -1.888 | 3.690 | 1.00 | 20.47 |
| ATOM | 1898 | O | ASP | 1682 | 19.172 | -1.984 | 4.906 | 1.00 | 21.83 |
| ATOM | 1899 | N | VAL | 1683 | 19.480 | -2.746 | 2.806 | 1.00 | 20.14 |
| ATOM | 1901 | CA | VAL | 1683 | 20.340 | -3.856 | 3.179 | 1.00 | 20.49 |
| ATOM | 1902 | CB | VAL | 1683 | 20.493 | -4.842 | 2.003 | 1.00 | 22.38 |
| ATOM | 1903 | CG1 | VAL | 1683 | 21.757 | -5.691 | 2.159 | 1.00 | 19.57 |
| ATOM | 1904 | CG2 | VAL | 1683 | 19.264 | -5.740 | 1.942 | 1.00 | 22.35 |
| ATOM | 1905 | C | VAL | 1683 | 21.677 | -3.315 | 3.683 | 1.00 | 20.22 |
| ATOM | 1906 | O | VAL | 1683 | 22.202 | -3.789 | 4.684 | 1.00 | 21.41 |
| ATOM | 1907 | N | TRP | 1684 | 22.210 | -2.311 | 3.003 | 1.00 | 21.33 |
| ATOM | 1909 | CA | TRP | 1684 | 23.440 | -1.666 | 3.449 | 1.00 | 22.21 |
| ATOM | 1910 | CB | TRP | 1684 | 23.768 | -0.473 | 2.540 | 1.00 | 18.78 |
| ATOM | 1911 | CG | TRP | 1684 | 24.924 | 0.391 | 3.037 | 1.00 | 22.80 |
| ATOM | 1912 | CD2 | TRP | 1684 | 26.237 | 0.477 | 2.472 | 1.00 | 24.60 |
| ATOM | 1913 | CE2 | TRP | 1684 | 26.989 | 1.364 | 3.286 | 1.00 | 24.34 |
| ATOM | 1914 | CE3 | TRP | 1684 | 26.853 | -0.099 | 1.352 | 1.00 | 24.32 |
| ATOM | 1915 | CD1 | TRP | 1684 | 24.933 | 1.208 | 4.138 | 1.00 | 22.28 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1916 | NE1 | TRP | 1684 | 26.169 | 1.791 | 4.297 | 1.00 | 22.32 |
| ATOM | 1918 | CZ2 | TRP | 1684 | 28.324 | 1.669 | 3.022 | 1.00 | 24.77 |
| ATOM | 1919 | CZ3 | TRP | 1684 | 28.193 | 0.213 | 1.090 | 1.00 | 24.46 |
| ATOM | 1920 | CH2 | TRP | 1684 | 28.906 | 1.088 | 1.918 | 1.00 | 24.00 |
| ATOM | 1921 | C | TRP | 1684 | 23.198 | -1.183 | 4.899 | 1.00 | 23.26 |
| ATOM | 1922 | O | TRP | 1684 | 23.982 | -1.475 | 5.805 | 1.00 | 24.52 |
| ATOM | 1923 | N | SER | 1685 | 22.108 | -0.447 | 5.113 | 1.00 | 22.88 |
| ATOM | 1925 | CA | SER | 1685 | 21.744 | 0.057 | 6.444 | 1.00 | 24.01 |
| ATOM | 1926 | CB | SER | 1685 | 20.398 | 0.783 | 6.385 | 1.00 | 21.90 |
| ATOM | 1927 | OG | SER | 1685 | 20.424 | 1.787 | 5.388 | 1.00 | 24.75 |
| ATOM | 1929 | C | SER | 1685 | 21.659 | -1.087 | 7.464 | 1.00 | 24.28 |
| ATOM | 1930 | O | SER | 1685 | 22.077 | -0.933 | 8.625 | 1.00 | 23.94 |
| ATOM | 1931 | N | PHE | 1686 | 21.099 | -2.221 | 7.037 | 1.00 | 23.20 |
| ATOM | 1933 | CA | PHE | 1686 | 20.993 | -3.393 | 7.898 | 1.00 | 23.87 |
| ATOM | 1934 | CB | PHE | 1686 | 20.216 | -4.519 | 7.216 | 1.00 | 19.56 |
| ATOM | 1935 | CG | PHE | 1686 | 20.062 | -5.734 | 8.075 | 1.00 | 22.19 |
| ATOM | 1936 | CD1 | PHE | 1686 | 19.240 | -5.701 | 9.203 | 1.00 | 21.55 |
| ATOM | 1937 | CD2 | PHE | 1686 | 20.773 | -6.899 | 7.793 | 1.00 | 21.94 |
| ATOM | 1938 | CE1 | PHE | 1686 | 19.125 | -6.801 | 10.033 | 1.00 | 21.66 |
| ATOM | 1939 | CE2 | PHE | 1686 | 20.663 | -8.012 | 8.623 | 1.00 | 22.47 |
| ATOM | 1940 | CZ | PHE | 1686 | 19.842 | -7.961 | 9.743 | 1.00 | 23.14 |
| ATOM | 1941 | C | PHE | 1686 | 22.389 | -3.890 | 8.300 | 1.00 | 22.62 |
| ATOM | 1942 | O | PHE | 1686 | 22.579 | -4.424 | 9.407 | 1.00 | 23.09 |
| ATOM | 1943 | N | GLY | 1687 | 23.354 | -3.726 | 7.401 | 1.00 | 23.50 |
| ATOM | 1945 | CA | GLY | 1687 | 24.718 | -4.110 | 7.721 | 1.00 | 23.83 |
| ATOM | 1946 | C | GLY | 1687 | 25.230 | -3.247 | 8.867 | 1.00 | 21.95 |
| ATOM | 1947 | O | GLY | 1687 | 25.901 | -3.749 | 9.778 | 1.00 | 23.76 |
| ATOM | 1948 | N | VAL | 1688 | 24.928 | -1.947 | 8.817 | 1.00 | 20.60 |
| ATOM | 1950 | CA | VAL | 1688 | 25.331 | -1.009 | 9.877 | 1.00 | 22.34 |
| ATOM | 1951 | CB | VAL | 1688 | 25.020 | 0.481 | 9.488 | 1.00 | 20.94 |
| ATOM | 1952 | CG1 | VAL | 1688 | 25.547 | 1.438 | 10.543 | 1.00 | 21.65 |
| ATOM | 1953 | CG2 | VAL | 1688 | 25.675 | 0.832 | 8.160 | 1.00 | 22.71 |
| ATOM | 1954 | C | VAL | 1688 | 24.598 | -1.400 | 11.182 | 1.00 | 22.71 |
| ATOM | 1955 | O | VAL | 1688 | 25.199 | -1.479 | 12.255 | 1.00 | 22.78 |
| ATOM | 1956 | N | LEU | 1689 | 23.310 | -1.706 | 11.082 | 1.00 | 22.81 |
| ATOM | 1958 | CA | LEU | 1689 | 22.534 | -2.111 | 12.253 | 1.00 | 25.21 |
| ATOM | 1959 | CB | LEU | 1689 | 21.064 | -2.357 | 11.866 | 1.00 | 25.78 |
| ATOM | 1960 | CG | LEU | 1689 | 20.006 | -2.491 | 12.976 | 1.00 | 29.18 |
| ATOM | 1961 | CD1 | LEU | 1689 | 18.643 | -2.109 | 12.408 | 1.00 | 28.57 |
| ATOM | 1962 | CD2 | LEU | 1689 | 19.959 | -3.895 | 13.553 | 1.00 | 26.77 |
| ATOM | 1963 | C | LEU | 1689 | 23.158 | -3.375 | 12.871 | 1.00 | 25.88 |
| ATOM | 1964 | O | LEU | 1689 | 23.249 | -3.483 | 14.099 | 1.00 | 26.50 |
| ATOM | 1965 | N | LEU | 1690 | 23.588 | -4.323 | 12.031 | 1.00 | 25.84 |
| ATOM | 1967 | CA | LEU | 1690 | 24.221 | -5.544 | 12.523 | 1.00 | 24.43 |
| ATOM | 1968 | CB | LEU | 1690 | 24.669 | -6.444 | 11.377 | 1.00 | 26.35 |
| ATOM | 1969 | CG | LEU | 1690 | 23.672 | -7.309 | 10.604 | 1.00 | 26.57 |
| ATOM | 1970 | CD1 | LEU | 1690 | 24.415 | -7.962 | 9.446 | 1.00 | 26.33 |
| ATOM | 1971 | CD2 | LEU | 1690 | 23.042 | -8.380 | 11.502 | 1.00 | 24.66 |
| ATOM | 1972 | C | LEU | 1690 | 25.430 | -5.168 | 13.349 | 1.00 | 25.22 |
| ATOM | 1973 | O | LEU | 1690 | 25.646 | -5.706 | 14.435 | 1.00 | 24.84 |
| ATOM | 1974 | N | TRP | 1691 | 26.211 | -4.227 | 12.826 | 1.00 | 26.92 |
| ATOM | 1976 | CA | TRP | 1691 | 27.405 | -3.728 | 13.504 | 1.00 | 25.77 |
| ATOM | 1977 | CB | TRP | 1691 | 28.072 | -2.659 | 12.631 | 1.00 | 24.82 |
| ATOM | 1978 | CG | TRP | 1691 | 29.394 | -2.195 | 13.154 | 1.00 | 27.98 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1979 | CD2 | TRP | 1691 | 29.623 | -1.104 | 14.056 | 1.00 | 26.95 |
| ATOM | 1980 | CE2 | TRP | 1691 | 31.022 | -1.015 | 14.259 | 1.00 | 27.64 |
| ATOM | 1981 | CE3 | TRP | 1691 | 28.783 | -0.191 | 14.708 | 1.00 | 26.28 |
| ATOM | 1982 | CD1 | TRP | 1691 | 30.634 | -2.715 | 12.856 | 1.00 | 28.38 |
| ATOM | 1983 | NE1 | TRP | 1691 | 31.609 | -2.009 | 13.518 | 1.00 | 29.56 |
| ATOM | 1985 | CZ2 | TRP | 1691 | 31.599 | -0.045 | 15.086 | 1.00 | 27.78 |
| ATOM | 1986 | CZ3 | TRP | 1691 | 29.356 | 0.769 | 15.533 | 1.00 | 27.63 |
| ATOM | 1987 | CH2 | TRP | 1691 | 30.753 | 0.835 | 15.713 | 1.00 | 30.68 |
| ATOM | 1988 | C | TRP | 1691 | 27.025 | -3.147 | 14.876 | 1.00 | 26.38 |
| ATOM | 1989 | O | TRP | 1691 | 27.686 | -3.414 | 15.883 | 1.00 | 24.82 |
| ATOM | 1990 | N | GLU | 1692 | 25.926 | -2.393 | 14.916 | 1.00 | 27.62 |
| ATOM | 1992 | CA | GLU | 1692 | 25.442 | -1.790 | 16.162 | 1.00 | 27.02 |
| ATOM | 1993 | CB | GLU | 1692 | 24.193 | -0.963 | 15.919 | 1.00 | 29.27 |
| ATOM | 1994 | CG | GLU | 1692 | 24.345 | 0.236 | 15.028 | 1.00 | 24.77 |
| ATOM | 1995 | CD | GLU | 1692 | 23.046 | 0.992 | 14.962 | 1.00 | 25.98 |
| ATOM | 1996 | OE1 | GLU | 1692 | 22.238 | 0.694 | 14.058 | 1.00 | 22.29 |
| ATOM | 1997 | OE2 | GLU | 1692 | 22.803 | 1.837 | 15.850 | 1.00 | 25.12 |
| ATOM | 1998 | C | GLU | 1692 | 25.092 | -2.856 | 17.191 | 1.00 | 27.88 |
| ATOM | 1999 | O | GLU | 1692 | 25.333 | -2.673 | 18.379 | 1.00 | 30.18 |
| ATOM | 2000 | N | ILE | 1693 | 24.500 | -3.956 | 16.734 | 1.00 | 26.65 |
| ATOM | 2002 | CA | ILE | 1693 | 24.118 | -5.054 | 17.618 | 1.00 | 26.14 |
| ATOM | 2003 | CB | ILE | 1693 | 23.279 | -6.144 | 16.858 | 1.00 | 25.37 |
| ATOM | 2004 | CG2 | ILE | 1693 | 23.144 | -7.445 | 17.704 | 1.00 | 21.48 |
| ATOM | 2005 | CG1 | ILE | 1693 | 21.897 | -5.563 | 16.496 | 1.00 | 24.80 |
| ATOM | 2006 | CD1 | ILE | 1693 | 21.017 | -6.479 | 15.642 | 1.00 | 22.40 |
| ATOM | 2007 | C | ILE | 1693 | 25.345 | -5.698 | 18.239 | 1.00 | 27.17 |
| ATOM | 2008 | O | ILE | 1693 | 25.424 | -5.864 | 19.452 | 1.00 | 27.30 |
| ATOM | 2009 | N | PHE | 1694 | 26.329 | -6.017 | 17.414 | 1.00 | 29.98 |
| ATOM | 2011 | CA | PHE | 1694 | 27.518 | -6.674 | 17.925 | 1.00 | 30.61 |
| ATOM | 2012 | CB | PHE | 1694 | 28.140 | -7.556 | 16.843 | 1.00 | 28.30 |
| ATOM | 2013 | CG | PHE | 1694 | 27.197 | -8.611 | 16.353 | 1.00 | 30.91 |
| ATOM | 2014 | CD1 | PHE | 1694 | 26.627 | -8.526 | 15.088 | 1.00 | 34.46 |
| ATOM | 2015 | CD2 | PHE | 1694 | 26.743 | -9.601 | 17.224 | 1.00 | 32.71 |
| ATOM | 2016 | CE1 | PHE | 1694 | 25.622 | -9.409 | 14.701 | 1.00 | 34.24 |
| ATOM | 2017 | CE2 | PHE | 1694 | 25.737 | -10.490 | 16.844 | 1.00 | 32.44 |
| ATOM | 2018 | CZ | PHE | 1694 | 25.170 | -10.387 | 15.592 | 1.00 | 32.70 |
| ATOM | 2019 | C | PHE | 1694 | 28.512 | -5.796 | 18.689 | 1.00 | 31.74 |
| ATOM | 2020 | O | PHE | 1694 | 29.469 | -6.299 | 19.276 | 1.00 | 35.15 |
| ATOM | 2021 | N | THR | 1695 | 28.275 | -4.489 | 18.698 | 1.00 | 31.12 |
| ATOM | 2023 | CA | THR | 1695 | 29.101 | -3.575 | 19.473 | 1.00 | 29.96 |
| ATOM | 2024 | CB | THR | 1695 | 29.532 | -2.351 | 18.657 | 1.00 | 28.09 |
| ATOM | 2025 | OG1 | THR | 1695 | 28.373 | -1.685 | 18.150 | 1.00 | 30.65 |
| ATOM | 2027 | CG2 | THR | 1695 | 30.450 | -2.767 | 17.510 | 1.00 | 23.37 |
| ATOM | 2028 | C | THR | 1695 | 28.240 | -3.128 | 20.664 | 1.00 | 30.01 |
| ATOM | 2029 | O | THR | 1695 | 28.617 | -2.233 | 21.427 | 1.00 | 31.14 |
| ATOM | 2030 | N | LEU | 1696 | 27.078 | -3.766 | 20.797 | 1.00 | 27.96 |
| ATOM | 2032 | CA | LEU | 1696 | 26.113 | -3.490 | 21.862 | 1.00 | 30.25 |
| ATOM | 2033 | CB | LEU | 1696 | 26.633 | -3.985 | 23.216 | 1.00 | 33.54 |
| ATOM | 2034 | CG | LEU | 1696 | 26.899 | -5.482 | 23.339 | 1.00 | 32.61 |
| ATOM | 2035 | CD1 | LEU | 1696 | 27.473 | -5.777 | 24.711 | 1.00 | 33.54 |
| ATOM | 2036 | CD2 | LEU | 1696 | 25.602 | -6.233 | 23.126 | 1.00 | 36.37 |
| ATOM | 2037 | C | LEU | 1696 | 25.717 | -2.031 | 21.958 | 1.00 | 28.19 |
| ATOM | 2038 | O | LEU | 1696 | 25.792 | -1.431 | 23.018 | 1.00 | 29.18 |
| ATOM | 2039 | N | GLY | 1697 | 25.251 | -1.472 | 20.853 | 1.00 | 28.24 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2041 | CA | GLY | 1697 | 24.851 | -0.082 | 20.858 | 1.00 | 28.29 |
| ATOM | 2042 | C | GLY | 1697 | 25.990 | 0.845 | 20.499 | 1.00 | 27.68 |
| ATOM | 2043 | O | GLY | 1697 | 25.960 | 2.022 | 20.846 | 1.00 | 29.79 |
| ATOM | 2044 | N | GLY | 1698 | 26.986 | 0.324 | 19.790 | 1.00 | 29.23 |
| ATOM | 2046 | CA | GLY | 1698 | 28.115 | 1.143 | 19.396 | 1.00 | 30.79 |
| ATOM | 2047 | C | GLY | 1698 | 27.743 | 2.212 | 18.388 | 1.00 | 32.38 |
| ATOM | 2048 | O | GLY | 1698 | 26.817 | 2.044 | 17.601 | 1.00 | 33.26 |
| ATOM | 2049 | N | SER | 1699 | 28.480 | 3.314 | 18.411 | 1.00 | 30.81 |
| ATOM | 2051 | CA | SER | 1699 | 28.268 | 4.437 | 17.510 | 1.00 | 32.03 |
| ATOM | 2052 | CB | SER | 1699 | 28.528 | 5.728 | 18.288 | 1.00 | 34.81 |
| ATOM | 2053 | OG | SER | 1699 | 28.559 | 6.862 | 17.440 | 1.00 | 40.03 |
| ATOM | 2055 | C | SER | 1699 | 29.198 | 4.325 | 16.282 | 1.00 | 32.20 |
| ATOM | 2056 | O | SER | 1699 | 30.428 | 4.325 | 16.408 | 1.00 | 31.67 |
| ATOM | 2057 | N | PRO | 1700 | 28.620 | 4.148 | 15.082 | 1.00 | 32.62 |
| ATOM | 2058 | CD | PRO | 1700 | 27.178 | 4.142 | 14.773 | 1.00 | 34.19 |
| ATOM | 2059 | CA | PRO | 1700 | 29.422 | 4.028 | 13.856 | 1.00 | 31.76 |
| ATOM | 2060 | CB | PRO | 1700 | 28.357 | 3.830 | 12.759 | 1.00 | 32.04 |
| ATOM | 2061 | CG | PRO | 1700 | 27.145 | 3.351 | 13.502 | 1.00 | 33.17 |
| ATOM | 2062 | C | PRO | 1700 | 30.214 | 5.309 | 13.609 | 1.00 | 28.70 |
| ATOM | 2063 | O | PRO | 1700 | 29.715 | 6.391 | 13.871 | 1.00 | 28.57 |
| ATOM | 2064 | N | TYR | 1701 | 31.459 | 5.181 | 13.164 | 1.00 | 28.61 |
| ATOM | 2066 | CA | TYR | 1701 | 32.311 | 6.338 | 12.870 | 1.00 | 29.92 |
| ATOM | 2067 | CB | TYR | 1701 | 31.920 | 6.946 | 11.510 | 1.00 | 30.15 |
| ATOM | 2068 | CG | TYR | 1701 | 31.965 | 5.994 | 10.339 | 1.00 | 36.17 |
| ATOM | 2069 | CD1 | TYR | 1701 | 30.799 | 5.630 | 9.664 | 1.00 | 39.26 |
| ATOM | 2070 | CE1 | TYR | 1701 | 30.839 | 4.767 | 8.571 | 1.00 | 41.51 |
| ATOM | 2071 | CD2 | TYR | 1701 | 33.176 | 5.467 | 9.893 | 1.00 | 37.48 |
| ATOM | 2072 | CE2 | TYR | 1701 | 33.229 | 4.607 | 8.805 | 1.00 | 42.94 |
| ATOM | 2073 | CZ | TYR | 1701 | 32.059 | 4.263 | 8.146 | 1.00 | 45.72 |
| ATOM | 2074 | OH | TYR | 1701 | 32.110 | 3.431 | 7.043 | 1.00 | 53.99 |
| ATOM | 2076 | C | TYR | 1701 | 32.279 | 7.448 | 13.941 | 1.00 | 31.09 |
| ATOM | 2077 | O | TYR | 1701 | 31.935 | 8.592 | 13.649 | 1.00 | 31.93 |
| ATOM | 2078 | N | PRO | 1702 | 32.649 | 7.135 | 15.189 | 1.00 | 34.66 |
| ATOM | 2079 | CD | PRO | 1702 | 33.212 | 5.879 | 15.708 | 1.00 | 36.83 |
| ATOM | 2080 | CA | PRO | 1702 | 32.631 | 8.173 | 16.231 | 1.00 | 33.54 |
| ATOM | 2081 | CB | PRO | 1702 | 33.116 | 7.432 | 17.479 | 1.00 | 32.18 |
| ATOM | 2082 | CG | PRO | 1702 | 32.903 | 6.001 | 17.175 | 1.00 | 40.82 |
| ATOM | 2083 | C | PRO | 1702 | 33.628 | 9.274 | 15.883 | 1.00 | 34.78 |
| ATOM | 2084 | O | PRO | 1702 | 34.750 | 8.981 | 15.455 | 1.00 | 33.97 |
| ATOM | 2085 | N | GLY | 1703 | 33.220 | 10.528 | 16.074 | 1.00 | 36.45 |
| ATOM | 2087 | CA | GLY | 1703 | 34.085 | 11.667 | 15.788 | 1.00 | 34.40 |
| ATOM | 2088 | C | GLY | 1703 | 34.245 | 12.006 | 14.317 | 1.00 | 34.34 |
| ATOM | 2089 | O | GLY | 1703 | 34.977 | 12.933 | 13.969 | 1.00 | 34.20 |
| ATOM | 2090 | N | VAL | 1704 | 33.552 | 11.275 | 13.445 | 1.00 | 35.02 |
| ATOM | 2092 | CA | VAL | 1704 | 33.641 | 11.512 | 12.007 | 1.00 | 32.77 |
| ATOM | 2093 | CB | VAL | 1704 | 33.614 | 10.176 | 11.221 | 1.00 | 31.32 |
| ATOM | 2094 | CG1 | VAL | 1704 | 33.628 | 10.435 | 9.709 | 1.00 | 31.46 |
| ATOM | 2095 | CG2 | VAL | 1704 | 34.796 | 9.297 | 11.637 | 1.00 | 27.62 |
| ATOM | 2096 | C | VAL | 1704 | 32.510 | 12.410 | 11.513 | 1.00 | 33.35 |
| ATOM | 2097 | O | VAL | 1704 | 31.337 | 12.070 | 11.640 | 1.00 | 33.94 |
| ATOM | 2098 | N | PRO | 1705 | 32.849 | 13.589 | 10.974 | 1.00 | 32.43 |
| ATOM | 2099 | CD | PRO | 1705 | 34.181 | 14.221 | 10.949 | 1.00 | 32.77 |
| ATOM | 2100 | CA | PRO | 1705 | 31.826 | 14.505 | 10.472 | 1.00 | 33.61 |
| ATOM | 2101 | CB | PRO | 1705 | 32.545 | 15.853 | 10.509 | 1.00 | 33.21 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2102 | CG | PRO | 1705 | 33.935 | 15.482 | 10.141 | 1.00 | 35.53 |
| ATOM | 2103 | C | PRO | 1705 | 31.395 | 14.138 | 9.052 | 1.00 | 33.91 |
| ATOM | 2104 | O | PRO | 1705 | 32.113 | 13.409 | 8.354 | 1.00 | 32.65 |
| ATOM | 2105 | N | VAL | 1706 | 30.255 | 14.684 | 8.619 | 1.00 | 33.82 |
| ATOM | 2107 | CA | VAL | 1706 | 29.689 | 14.447 | 7.280 | 1.00 | 33.97 |
| ATOM | 2108 | CB | VAL | 1706 | 28.617 | 15.513 | 6.943 | 1.00 | 37.41 |
| ATOM | 2109 | CG1 | VAL | 1706 | 28.045 | 15.282 | 5.556 | 1.00 | 41.12 |
| ATOM | 2110 | CG2 | VAL | 1706 | 27.507 | 15.484 | 7.971 | 1.00 | 38.89 |
| ATOM | 2111 | C | VAL | 1706 | 30.712 | 14.428 | 6.135 | 1.00 | 32.32 |
| ATOM | 2112 | O | VAL | 1706 | 30.819 | 13.450 | 5.398 | 1.00 | 32.58 |
| ATOM | 2113 | N | GLU | 1707 | 31.477 | 15.504 | 6.004 | 1.00 | 31.15 |
| ATOM | 2115 | CA | GLU | 1707 | 32.478 | 15.630 | 4.956 | 1.00 | 29.82 |
| ATOM | 2116 | CB | GLU | 1707 | 33.172 | 16.989 | 5.048 | 1.00 | 30.05 |
| ATOM | 2117 | C | GLU | 1707 | 33.531 | 14.541 | 4.959 | 1.00 | 28.52 |
| ATOM | 2118 | O | GLU | 1707 | 33.995 | 14.134 | 3.896 | 1.00 | 30.85 |
| ATOM | 2119 | N | GLU | 1708 | 33.958 | 14.110 | 6.143 | 1.00 | 28.70 |
| ATOM | 2121 | CA | GLU | 1708 | 34.978 | 13.073 | 6.235 | 1.00 | 29.50 |
| ATOM | 2122 | CB | GLU | 1708 | 35.590 | 13.010 | 7.641 | 1.00 | 31.28 |
| ATOM | 2123 | CG | GLU | 1708 | 36.281 | 14.289 | 8.103 | 1.00 | 41.63 |
| ATOM | 2124 | CD | GLU | 1708 | 37.454 | 14.718 | 7.237 | 1.00 | 49.91 |
| ATOM | 2125 | OE1 | GLU | 1708 | 38.020 | 13.876 | 6.498 | 1.00 | 53.57 |
| ATOM | 2126 | OE2 | GLU | 1708 | 37.821 | 15.916 | 7.308 | 1.00 | 58.45 |
| ATOM | 2127 | C | GLU | 1708 | 34.365 | 11.730 | 5.878 | 1.00 | 30.00 |
| ATOM | 2128 | O | GLU | 1708 | 35.016 | 10.874 | 5.257 | 1.00 | 28.43 |
| ATOM | 2129 | N | LEU | 1709 | 33.103 | 11.559 | 6.257 | 1.00 | 30.08 |
| ATOM | 2131 | CA | LEU | 1709 | 32.392 | 10.324 | 5.964 | 1.00 | 29.19 |
| ATOM | 2132 | CB | LEU | 1709 | 30.995 | 10.347 | 6.592 | 1.00 | 28.97 |
| ATOM | 2133 | CG | LEU | 1709 | 30.109 | 9.186 | 6.137 | 1.00 | 30.66 |
| ATOM | 2134 | CD1 | LEU | 1709 | 30.664 | 7.866 | 6.659 | 1.00 | 29.24 |
| ATOM | 2135 | CD2 | LEU | 1709 | 28.684 | 9.403 | 6.593 | 1.00 | 29.29 |
| ATOM | 2136 | C | LEU | 1709 | 32.294 | 10.130 | 4.449 | 1.00 | 28.26 |
| ATOM | 2137 | O | LEU | 1709 | 32.450 | 9.011 | 3.948 | 1.00 | 28.86 |
| ATOM | 2138 | N | PHE | 1710 | 32.016 | 11.220 | 3.735 | 1.00 | 26.86 |
| ATOM | 2140 | CA | PHE | 1710 | 31.903 | 11.192 | 2.285 | 1.00 | 28.86 |
| ATOM | 2141 | CB | PHE | 1710 | 31.632 | 12.593 | 1.743 | 1.00 | 31.88 |
| ATOM | 2142 | CG | PHE | 1710 | 30.249 | 13.095 | 2.014 | 1.00 | 37.62 |
| ATOM | 2143 | CD1 | PHE | 1710 | 29.265 | 12.247 | 2.509 | 1.00 | 42.63 |
| ATOM | 2144 | CD2 | PHE | 1710 | 29.931 | 14.424 | 1.792 | 1.00 | 43.53 |
| ATOM | 2145 | CE1 | PHE | 1710 | 27.977 | 12.718 | 2.783 | 1.00 | 45.99 |
| ATOM | 2146 | CE2 | PHE | 1710 | 28.648 | 14.905 | 2.061 | 1.00 | 46.25 |
| ATOM | 2147 | CZ | PHE | 1710 | 27.670 | 14.045 | 2.559 | 1.00 | 44.45 |
| ATOM | 2148 | C | PHE | 1710 | 33.193 | 10.660 | 1.681 | 1.00 | 30.42 |
| ATOM | 2149 | O | PHE | 1710 | 33.174 | 9.807 | 0.792 | 1.00 | 29.01 |
| ATOM | 2150 | N | LYS | 1711 | 34.309 | 11.152 | 2.212 | 1.00 | 30.64 |
| ATOM | 2152 | CA | LYS | 1711 | 35.650 | 10.762 | 1.786 | 1.00 | 32.89 |
| ATOM | 2153 | CB | LYS | 1711 | 36.670 | 11.655 | 2.502 | 1.00 | 37.91 |
| ATOM | 2154 | CG | LYS | 1711 | 38.108 | 11.479 | 2.088 | 1.00 | 42.99 |
| ATOM | 2155 | CD | LYS | 1711 | 38.976 | 12.528 | 2.752 | 1.00 | 47.45 |
| ATOM | 2156 | CE | LYS | 1711 | 40.380 | 12.505 | 2.182 | 1.00 | 52.35 |
| ATOM | 2157 | NZ | LYS | 1711 | 41.104 | 11.272 | 2.587 | 1.00 | 58.47 |
| ATOM | 2161 | C | LYS | 1711 | 35.913 | 9.273 | 2.071 | 1.00 | 32.23 |
| ATOM | 2162 | O | LYS | 1711 | 36.445 | 8.559 | 1.216 | 1.00 | 30.79 |
| ATOM | 2163 | N | LEU | 1712 | 35.533 | 8.807 | 3.264 | 1.00 | 31.37 |
| ATOM | 2165 | CA | LEU | 1712 | 35.704 | 7.399 | 3.630 | 1.00 | 29.46 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2166 | CB | LEU | 1712 | 35.220 | 7.117 | 5.065 | 1.00 | 28.57 |
| ATOM | 2167 | CG | LEU | 1712 | 36.045 | 7.662 | 6.242 | 1.00 | 30.18 |
| ATOM | 2168 | CD1 | LEU | 1712 | 35.395 | 7.349 | 7.569 | 1.00 | 26.92 |
| ATOM | 2169 | CD2 | LEU | 1712 | 37.452 | 7.083 | 6.210 | 1.00 | 30.88 |
| ATOM | 2170 | C | LEU | 1712 | 34.922 | 6.539 | 2.651 | 1.00 | 28.99 |
| ATOM | 2171 | O | LEU | 1712 | 35.438 | 5.551 | 2.136 | 1.00 | 30.73 |
| ATOM | 2172 | N | LEU | 1713 | 33.675 | 6.915 | 2.388 | 1.00 | 30.13 |
| ATOM | 2174 | CA | LEU | 1713 | 32.851 | 6.158 | 1.456 | 1.00 | 32.10 |
| ATOM | 2175 | CB | LEU | 1713 | 31.411 | 6.685 | 1.443 | 1.00 | 35.23 |
| ATOM | 2176 | CG | LEU | 1713 | 30.612 | 6.292 | 2.691 | 1.00 | 37.47 |
| ATOM | 2177 | CD1 | LEU | 1713 | 29.265 | 6.982 | 2.720 | 1.00 | 40.85 |
| ATOM | 2178 | CD2 | LEU | 1713 | 30.447 | 4.788 | 2.723 | 1.00 | 39.61 |
| ATOM | 2179 | C | LEU | 1713 | 33.441 | 6.147 | 0.047 | 1.00 | 32.70 |
| ATOM | 2180 | O | LEU | 1713 | 33.548 | 5.090 | -0.578 | 1.00 | 31.86 |
| ATOM | 2181 | N | LYS | 1714 | 33.859 | 7.309 | -0.444 | 1.00 | 32.42 |
| ATOM | 2183 | CA | LYS | 1714 | 34.440 | 7.387 | -1.776 | 1.00 | 32.56 |
| ATOM | 2184 | CB | LYS | 1714 | 34.826 | 8.824 | -2.112 | 1.00 | 33.02 |
| ATOM | 2185 | CG | LYS | 1714 | 33.640 | 9.736 | -2.297 | 1.00 | 35.56 |
| ATOM | 2186 | CD | LYS | 1714 | 32.736 | 9.235 | -3.396 | 1.00 | 37.94 |
| ATOM | 2187 | CE | LYS | 1714 | 31.635 | 10.246 | -3.682 | 1.00 | 42.57 |
| ATOM | 2188 | NZ | LYS | 1714 | 30.727 | 9.805 | -4.779 | 1.00 | 47.40 |
| ATOM | 2192 | C | LYS | 1714 | 35.664 | 6.488 | -1.885 | 1.00 | 35.36 |
| ATOM | 2193 | O | LYS | 1714 | 35.927 | 5.898 | -2.937 | 1.00 | 36.68 |
| ATOM | 2194 | N | GLU | 1715 | 36.376 | 6.338 | -0.775 | 1.00 | 34.51 |
| ATOM | 2196 | CA | GLU | 1715 | 37.577 | 5.527 | -0.749 | 1.00 | 35.31 |
| ATOM | 2197 | CB | GLU | 1715 | 38.566 | 6.125 | 0.250 | 1.00 | 37.07 |
| ATOM | 2198 | CG | GLU | 1715 | 38.967 | 7.537 | -0.163 | 1.00 | 43.62 |
| ATOM | 2199 | CD | GLU | 1715 | 39.735 | 8.310 | 0.893 | 1.00 | 49.75 |
| ATOM | 2200 | OE1 | GLU | 1715 | 39.906 | 7.814 | 2.029 | 1.00 | 49.71 |
| ATOM | 2201 | OE2 | GLU | 1715 | 40.163 | 9.442 | 0.572 | 1.00 | 55.13 |
| ATOM | 2202 | C | GLU | 1715 | 37.321 | 4.048 | -0.487 | 1.00 | 34.08 |
| ATOM | 2203 | O | GLU | 1715 | 38.259 | 3.260 | -0.438 | 1.00 | 34.82 |
| ATOM | 2204 | N | GLY | 1716 | 36.049 | 3.674 | -0.366 | 1.00 | 31.53 |
| ATOM | 2206 | CA | GLY | 1716 | 35.695 | 2.288 | -0.133 | 1.00 | 27.58 |
| ATOM | 2207 | C | GLY | 1716 | 35.966 | 1.765 | 1.262 | 1.00 | 28.60 |
| ATOM | 2208 | O | GLY | 1716 | 36.069 | 0.560 | 1.464 | 1.00 | 27.81 |
| ATOM | 2209 | N | HIS | 1717 | 36.062 | 2.663 | 2.236 | 1.00 | 29.10 |
| ATOM | 2211 | CA | HIS | 1717 | 36.319 | 2.263 | 3.617 | 1.00 | 29.30 |
| ATOM | 2212 | CB | HIS | 1717 | 36.501 | 3.510 | 4.486 | 1.00 | 30.54 |
| ATOM | 2213 | CG | HIS | 1717 | 36.788 | 3.213 | 5.930 | 1.00 | 32.88 |
| ATOM | 2214 | CD2 | HIS | 1717 | 37.961 | 3.023 | 6.586 | 1.00 | 32.21 |
| ATOM | 2215 | ND1 | HIS | 1717 | 35.798 | 3.108 | 6.881 | 1.00 | 34.22 |
| ATOM | 2217 | CE1 | HIS | 1717 | 36.342 | 2.865 | 8.061 | 1.00 | 31.51 |
| ATOM | 2218 | NE2 | HIS | 1717 | 37.651 | 2.809 | 7.907 | 1.00 | 31.94 |
| ATOM | 2220 | C | HIS | 1717 | 35.180 | 1.416 | 4.183 | 1.00 | 28.42 |
| ATOM | 2221 | O | HIS | 1717 | 34.017 | 1.666 | 3.885 | 1.00 | 30.71 |
| ATOM | 2222 | N | ARG | 1718 | 35.526 | 0.450 | 5.028 | 1.00 | 27.75 |
| ATOM | 2224 | CA | ARG | 1718 | 34.559 | -0.423 | 5.688 | 1.00 | 27.58 |
| ATOM | 2225 | CB | ARG | 1718 | 34.562 | -1.813 | 5.048 | 1.00 | 29.07 |
| ATOM | 2226 | CG | ARG | 1718 | 34.078 | -1.860 | 3.597 | 1.00 | 28.39 |
| ATOM | 2227 | CD | ARG | 1718 | 32.609 | -1.412 | 3.475 | 1.00 | 27.64 |
| ATOM | 2228 | NE | ARG | 1718 | 32.091 | -1.467 | 2.096 | 1.00 | 24.37 |
| ATOM | 2230 | CZ | ARG | 1718 | 32.173 | -0.476 | 1.210 | 1.00 | 24.26 |
| ATOM | 2231 | NH1 | ARG | 1718 | 32.768 | 0.668 | 1.532 | 1.00 | 23.98 |

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ATOM   2234  NH2  ARG  1718   31.595   -0.603    0.019  1.00  21.60
ATOM   2237  C    ARG  1718   35.005   -0.521    7.148  1.00  30.11
ATOM   2238  O    ARG  1718   36.201   -0.623    7.428  1.00  30.60
ATOM   2239  N    MET  1719   34.056   -0.430    8.074  1.00  30.69
ATOM   2241  CA   MET  1719   34.350   -0.490    9.501  1.00  31.77
ATOM   2242  CB   MET  1719   33.072   -0.302   10.335  1.00  34.56
ATOM   2243  CG   MET  1719   32.408    1.060   10.194  1.00  36.71
ATOM   2244  SD   MET  1719   31.015    1.307   11.314  1.00  38.66
ATOM   2245  CE   MET  1719   29.797    0.338   10.544  1.00  36.99
ATOM   2246  C    MET  1719   34.998   -1.810    9.854  1.00  30.20
ATOM   2247  O    MET  1719   34.802   -2.802    9.169  1.00  31.41
ATOM   2248  N    ASP  1720   35.778   -1.809   10.926  1.00  32.49
ATOM   2250  CA   ASP  1720   36.473   -3.008   11.385  1.00  33.60
ATOM   2251  CB   ASP  1720   37.593   -2.630   12.358  1.00  37.65
ATOM   2252  CG   ASP  1720   38.628   -1.688   11.747  1.00  44.69
ATOM   2253  OD1  ASP  1720   38.442   -1.223   10.596  1.00  50.97
ATOM   2254  OD2  ASP  1720   39.632   -1.398   12.443  1.00  48.67
ATOM   2255  C    ASP  1720   35.524   -3.977   12.079  1.00  31.26
ATOM   2256  O    ASP  1720   34.466   -3.581   12.561  1.00  32.69
ATOM   2257  N    LYS  1721   35.943   -5.231   12.191  1.00  32.76
ATOM   2259  CA   LYS  1721   35.133   -6.261   12.825  1.00  32.28
ATOM   2260  CB   LYS  1721   35.726   -7.649   12.575  1.00  33.63
ATOM   2261  CG   LYS  1721   34.854   -8.773   13.125  1.00  35.68
ATOM   2262  CD   LYS  1721   35.392  -10.126   12.784  1.00  36.22
ATOM   2263  CE   LYS  1721   36.054  -10.749   13.988  1.00  42.65
ATOM   2264  NZ   LYS  1721   36.354  -12.189   13.756  1.00  46.15
ATOM   2268  C    LYS  1721   35.039   -6.051   14.315  1.00  35.55
ATOM   2269  O    LYS  1721   36.064   -5.926   14.986  1.00  37.78
ATOM   2270  N    PRO  1722   33.807   -6.017   14.861  1.00  36.91
ATOM   2271  CD   PRO  1722   32.504   -6.105   14.179  1.00  34.43
ATOM   2272  CA   PRO  1722   33.630   -5.827   16.305  1.00  37.77
ATOM   2273  CB   PRO  1722   32.107   -5.846   16.465  1.00  36.32
ATOM   2274  CG   PRO  1722   31.603   -5.375   15.122  1.00  34.53
ATOM   2275  C    PRO  1722   34.246   -7.026   17.023  1.00  39.31
ATOM   2276  O    PRO  1722   34.274   -8.136   16.477  1.00  38.78
ATOM   2277  N    SER  1723   34.777   -6.820   18.222  1.00  42.72
ATOM   2279  CA   SER  1723   35.336   -7.954   18.940  1.00  45.01
ATOM   2280  CB   SER  1723   36.152   -7.508   20.160  1.00  46.88
ATOM   2281  OG   SER  1723   35.327   -7.027   21.208  1.00  53.47
ATOM   2283  C    SER  1723   34.088   -8.731   19.359  1.00  46.67
ATOM   2284  O    SER  1723   32.982   -8.172   19.417  1.00  46.21
ATOM   2285  N    ASN  1724   34.237  -10.025   19.590  1.00  47.80
ATOM   2287  CA   ASN  1724   33.092  -10.826   19.999  1.00  52.78
ATOM   2288  CB   ASN  1724   32.559  -10.319   21.355  1.00  57.86
ATOM   2289  CG   ASN  1724   33.679  -10.091   22.370  1.00  61.99
ATOM   2290  OD1  ASN  1724   34.531  -10.959   22.585  1.00  63.17
ATOM   2291  ND2  ASN  1724   33.712   -8.899   22.953  1.00  63.56
ATOM   2294  C    ASN  1724   32.015  -10.779   18.893  1.00  51.43
ATOM   2295  O    ASN  1724   30.859  -10.423   19.108  1.00  51.56
ATOM   2296  N    CYS  1725   32.454  -11.087   17.683  1.00  48.91
ATOM   2298  CA   CYS  1725   31.600  -11.136   16.508  1.00  45.62
ATOM   2299  CB   CYS  1725   31.526   -9.771   15.811  1.00  44.83
ATOM   2300  SG   CYS  1725   30.693   -9.816   14.194  1.00  41.83
ATOM   2301  C    CYS  1725   32.341  -12.135   15.640  1.00  42.30
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2302 | O | CYS | 1725 | 33.566 | -12.045 | 15.493 | 1.00 | 44.63 |
| ATOM | 2303 | N | THR | 1726 | 31.627 | -13.134 | 15.141 | 1.00 | 37.46 |
| ATOM | 2305 | CA | THR | 1726 | 32.259 | -14.153 | 14.320 | 1.00 | 35.29 |
| ATOM | 2306 | CB | THR | 1726 | 31.339 | -15.367 | 14.132 | 1.00 | 33.44 |
| ATOM | 2307 | OG1 | THR | 1726 | 30.109 | -14.952 | 13.523 | 1.00 | 34.77 |
| ATOM | 2309 | CG2 | THR | 1726 | 31.070 | -16.019 | 15.454 | 1.00 | 30.22 |
| ATOM | 2310 | C | THR | 1726 | 32.668 | -13.622 | 12.963 | 1.00 | 33.53 |
| ATOM | 2311 | O | THR | 1726 | 32.158 | -12.593 | 12.518 | 1.00 | 32.93 |
| ATOM | 2312 | N | ASN | 1727 | 33.619 | -14.294 | 12.319 | 1.00 | 32.72 |
| ATOM | 2314 | CA | ASN | 1727 | 34.030 | -13.867 | 10.983 | 1.00 | 35.91 |
| ATOM | 2315 | CB | ASN | 1727 | 35.166 | -14.724 | 10.422 | 1.00 | 40.64 |
| ATOM | 2316 | CG | ASN | 1727 | 36.463 | -14.533 | 11.168 | 1.00 | 46.52 |
| ATOM | 2317 | OD1 | ASN | 1727 | 37.047 | -13.453 | 11.158 | 1.00 | 49.98 |
| ATOM | 2318 | ND2 | ASN | 1727 | 36.931 | -15.592 | 11.814 | 1.00 | 49.04 |
| ATOM | 2321 | C | ASN | 1727 | 32.824 | -14.006 | 10.058 | 1.00 | 34.27 |
| ATOM | 2322 | O | ASN | 1727 | 32.681 | -13.236 | 9.116 | 1.00 | 32.96 |
| ATOM | 2323 | N | GLU | 1728 | 31.969 | -14.997 | 10.326 | 1.00 | 32.49 |
| ATOM | 2325 | CA | GLU | 1728 | 30.778 | -15.235 | 9.510 | 1.00 | 31.99 |
| ATOM | 2326 | CB | GLU | 1728 | 30.064 | -16.504 | 9.975 | 1.00 | 34.15 |
| ATOM | 2327 | CG | GLU | 1728 | 28.836 | -16.866 | 9.156 | 1.00 | 35.63 |
| ATOM | 2328 | CD | GLU | 1728 | 28.187 | -18.169 | 9.608 | 1.00 | 39.72 |
| ATOM | 2329 | OE1 | GLU | 1728 | 28.200 | -18.463 | 10.824 | 1.00 | 42.25 |
| ATOM | 2330 | OE2 | GLU | 1728 | 27.654 | -18.896 | 8.742 | 1.00 | 39.87 |
| ATOM | 2331 | C | GLU | 1728 | 29.814 | -14.049 | 9.549 | 1.00 | 30.76 |
| ATOM | 2332 | O | GLU | 1728 | 29.309 | -13.602 | 8.512 | 1.00 | 29.58 |
| ATOM | 2333 | N | LEU | 1729 | 29.559 | -13.544 | 10.750 | 1.00 | 30.01 |
| ATOM | 2335 | CA | LEU | 1729 | 28.670 | -12.408 | 10.911 | 1.00 | 30.21 |
| ATOM | 2336 | CB | LEU | 1729 | 28.225 | -12.272 | 12.364 | 1.00 | 30.13 |
| ATOM | 2337 | CG | LEU | 1729 | 27.208 | -13.350 | 12.748 | 1.00 | 33.61 |
| ATOM | 2338 | CD1 | LEU | 1729 | 27.119 | -13.483 | 14.262 | 1.00 | 33.71 |
| ATOM | 2339 | CD2 | LEU | 1729 | 25.844 | -13.021 | 12.139 | 1.00 | 30.31 |
| ATOM | 2340 | C | LEU | 1729 | 29.316 | -11.133 | 10.390 | 1.00 | 30.26 |
| ATOM | 2341 | O | LEU | 1729 | 28.619 | -10.229 | 9.938 | 1.00 | 28.89 |
| ATOM | 2342 | N | TYR | 1730 | 30.648 | -11.063 | 10.435 | 1.00 | 28.91 |
| ATOM | 2344 | CA | TYR | 1730 | 31.343 | -9.893 | 9.912 | 1.00 | 28.91 |
| ATOM | 2345 | CB | TYR | 1730 | 32.804 | -9.861 | 10.359 | 1.00 | 29.09 |
| ATOM | 2346 | CG | TYR | 1730 | 33.537 | -8.639 | 9.857 | 1.00 | 30.15 |
| ATOM | 2347 | CD1 | TYR | 1730 | 33.037 | -7.358 | 10.103 | 1.00 | 29.97 |
| ATOM | 2348 | CE1 | TYR | 1730 | 33.688 | -6.227 | 9.626 | 1.00 | 28.99 |
| ATOM | 2349 | CD2 | TYR | 1730 | 34.716 | -8.757 | 9.119 | 1.00 | 29.24 |
| ATOM | 2350 | CE2 | TYR | 1730 | 35.386 | -7.620 | 8.632 | 1.00 | 28.25 |
| ATOM | 2351 | CZ | TYR | 1730 | 34.861 | -6.362 | 8.889 | 1.00 | 28.41 |
| ATOM | 2352 | OH | TYR | 1730 | 35.485 | -5.227 | 8.405 | 1.00 | 31.64 |
| ATOM | 2354 | C | TYR | 1730 | 31.260 | -9.943 | 8.379 | 1.00 | 27.10 |
| ATOM | 2355 | O | TYR | 1730 | 31.078 | -8.920 | 7.726 | 1.00 | 27.46 |
| ATOM | 2356 | N | MET | 1731 | 31.390 | -11.138 | 7.813 | 1.00 | 26.68 |
| ATOM | 2358 | CA | MET | 1731 | 31.298 | -11.315 | 6.372 | 1.00 | 28.68 |
| ATOM | 2359 | CB | MET | 1731 | 31.526 | -12.778 | 5.989 | 1.00 | 35.43 |
| ATOM | 2360 | CG | MET | 1731 | 31.158 | -13.087 | 4.545 | 1.00 | 46.19 |
| ATOM | 2361 | SD | MET | 1731 | 31.441 | -14.804 | 4.064 | 1.00 | 60.10 |
| ATOM | 2362 | CE | MET | 1731 | 32.603 | -14.550 | 2.678 | 1.00 | 58.31 |
| ATOM | 2363 | C | MET | 1731 | 29.917 | -10.858 | 5.912 | 1.00 | 27.42 |
| ATOM | 2364 | O | MET | 1731 | 29.782 | -10.227 | 4.871 | 1.00 | 30.80 |
| ATOM | 2365 | N | MET | 1732 | 28.893 | -11.191 | 6.688 | 1.00 | 28.53 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2367 | CA | MET | 1732 | 27.522 | -10.777 | 6.389 | 1.00 | 26.47 |
| ATOM | 2368 | CB | MET | 1732 | 26.562 | -11.308 | 7.458 | 1.00 | 25.79 |
| ATOM | 2369 | CG | MET | 1732 | 25.116 | -10.838 | 7.274 | 1.00 | 26.01 |
| ATOM | 2370 | SD | MET | 1732 | 24.004 | -11.550 | 8.469 | 1.00 | 26.22 |
| ATOM | 2371 | CE | MET | 1732 | 23.787 | -13.195 | 7.783 | 1.00 | 23.74 |
| ATOM | 2372 | C | MET | 1732 | 27.445 | -9.243 | 6.319 | 1.00 | 25.15 |
| ATOM | 2373 | O | MET | 1732 | 26.886 | -8.691 | 5.379 | 1.00 | 25.41 |
| ATOM | 2374 | N | MET | 1733 | 28.024 | -8.564 | 7.308 | 1.00 | 26.48 |
| ATOM | 2376 | CA | MET | 1733 | 28.057 | -7.104 | 7.331 | 1.00 | 27.09 |
| ATOM | 2377 | CB | MET | 1733 | 28.903 | -6.594 | 8.488 | 1.00 | 25.91 |
| ATOM | 2378 | CG | MET | 1733 | 28.235 | -6.556 | 9.824 | 1.00 | 31.64 |
| ATOM | 2379 | SD | MET | 1733 | 29.442 | -6.111 | 11.094 | 1.00 | 29.59 |
| ATOM | 2380 | CE | MET | 1733 | 28.886 | -7.126 | 12.420 | 1.00 | 28.14 |
| ATOM | 2381 | C | MET | 1733 | 28.720 | -6.613 | 6.056 | 1.00 | 28.43 |
| ATOM | 2382 | O | MET | 1733 | 28.185 | -5.753 | 5.372 | 1.00 | 31.37 |
| ATOM | 2383 | N | ARG | 1734 | 29.891 | -7.169 | 5.747 | 1.00 | 28.57 |
| ATOM | 2385 | CA | ARG | 1734 | 30.642 | -6.783 | 4.551 | 1.00 | 27.00 |
| ATOM | 2386 | CB | ARG | 1734 | 32.007 | -7.488 | 4.510 | 1.00 | 25.98 |
| ATOM | 2387 | CG | ARG | 1734 | 32.927 | -7.154 | 5.707 | 1.00 | 28.13 |
| ATOM | 2388 | CD | ARG | 1734 | 33.229 | -5.672 | 5.765 | 1.00 | 29.97 |
| ATOM | 2389 | NE | ARG | 1734 | 33.922 | -5.256 | 4.553 | 1.00 | 40.49 |
| ATOM | 2391 | CZ | ARG | 1734 | 35.238 | -5.361 | 4.363 | 1.00 | 43.95 |
| ATOM | 2392 | NH1 | ARG | 1734 | 36.023 | -5.853 | 5.318 | 1.00 | 41.81 |
| ATOM | 2395 | NH2 | ARG | 1734 | 35.760 | -5.048 | 3.184 | 1.00 | 46.20 |
| ATOM | 2398 | C | ARG | 1734 | 29.859 | -7.037 | 3.268 | 1.00 | 24.57 |
| ATOM | 2399 | O | ARG | 1734 | 29.992 | -6.290 | 2.314 | 1.00 | 24.94 |
| ATOM | 2400 | N | ASP | 1735 | 29.071 | -8.107 | 3.235 | 1.00 | 24.79 |
| ATOM | 2402 | CA | ASP | 1735 | 28.254 | -8.420 | 2.061 | 1.00 | 23.88 |
| ATOM | 2403 | CB | ASP | 1735 | 27.669 | -9.830 | 2.150 | 1.00 | 25.95 |
| ATOM | 2404 | CG | ASP | 1735 | 28.724 | -10.913 | 2.024 | 1.00 | 27.60 |
| ATOM | 2405 | OD1 | ASP | 1735 | 29.842 | -10.632 | 1.529 | 1.00 | 27.75 |
| ATOM | 2406 | OD2 | ASP | 1735 | 28.432 | -12.051 | 2.430 | 1.00 | 28.90 |
| ATOM | 2407 | C | ASP | 1735 | 27.139 | -7.396 | 1.941 | 1.00 | 22.61 |
| ATOM | 2408 | O | ASP | 1735 | 26.777 | -6.996 | 0.833 | 1.00 | 22.66 |
| ATOM | 2409 | N | CYS | 1736 | 26.611 | -6.965 | 3.085 | 1.00 | 20.61 |
| ATOM | 2411 | CA | CYS | 1736 | 25.561 | -5.952 | 3.109 | 1.00 | 23.63 |
| ATOM | 2412 | CB | CYS | 1736 | 25.007 | -5.767 | 4.534 | 1.00 | 21.98 |
| ATOM | 2413 | SG | CYS | 1736 | 23.934 | -7.126 | 5.111 | 1.00 | 22.95 |
| ATOM | 2414 | C | CYS | 1736 | 26.129 | -4.633 | 2.599 | 1.00 | 23.62 |
| ATOM | 2415 | O | CYS | 1736 | 25.403 | -3.797 | 2.047 | 1.00 | 22.15 |
| ATOM | 2416 | N | TRP | 1737 | 27.438 | -4.461 | 2.775 | 1.00 | 24.37 |
| ATOM | 2418 | CA | TRP | 1737 | 28.123 | -3.247 | 2.342 | 1.00 | 23.77 |
| ATOM | 2419 | CB | TRP | 1737 | 29.162 | -2.810 | 3.371 | 1.00 | 19.38 |
| ATOM | 2420 | CG | TRP | 1737 | 28.601 | -2.520 | 4.718 | 1.00 | 21.62 |
| ATOM | 2421 | CD2 | TRP | 1737 | 29.268 | -2.688 | 5.971 | 1.00 | 24.81 |
| ATOM | 2422 | CE2 | TRP | 1737 | 28.371 | -2.278 | 6.980 | 1.00 | 25.95 |
| ATOM | 2423 | CE3 | TRP | 1737 | 30.534 | -3.165 | 6.340 | 1.00 | 29.02 |
| ATOM | 2424 | CD1 | TRP | 1737 | 27.359 | -2.024 | 5.007 | 1.00 | 23.21 |
| ATOM | 2425 | NE1 | TRP | 1737 | 27.213 | -1.876 | 6.362 | 1.00 | 21.80 |
| ATOM | 2427 | CZ2 | TRP | 1737 | 28.710 | -2.305 | 8.347 | 1.00 | 26.68 |
| ATOM | 2428 | CZ3 | TRP | 1737 | 30.873 | -3.198 | 7.699 | 1.00 | 31.06 |
| ATOM | 2429 | CH2 | TRP | 1737 | 29.959 | -2.774 | 8.685 | 1.00 | 30.18 |
| ATOM | 2430 | C | TRP | 1737 | 28.788 | -3.372 | 0.978 | 1.00 | 24.88 |
| ATOM | 2431 | O | TRP | 1737 | 29.737 | -2.646 | 0.689 | 1.00 | 25.11 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2432 | N | HIS | 1738 | 28.303 | -4.278 | 0.132 | 1.00 | 25.27 |
| ATOM | 2434 | CA | HIS | 1738 | 28.888 | -4.406 | -1.191 | 1.00 | 24.27 |
| ATOM | 2435 | CB | HIS | 1738 | 28.280 | -5.573 | -1.986 | 1.00 | 25.24 |
| ATOM | 2436 | CG | HIS | 1738 | 29.179 | -6.073 | -3.081 | 1.00 | 26.28 |
| ATOM | 2437 | CD2 | HIS | 1738 | 29.727 | -5.437 | -4.147 | 1.00 | 25.67 |
| ATOM | 2438 | ND1 | HIS | 1738 | 29.697 | -7.352 | -3.098 | 1.00 | 27.55 |
| ATOM | 2440 | CE1 | HIS | 1738 | 30.528 | -7.478 | -4.117 | 1.00 | 27.51 |
| ATOM | 2441 | NE2 | HIS | 1738 | 30.564 | -6.329 | -4.770 | 1.00 | 30.93 |
| ATOM | 2443 | C | HIS | 1738 | 28.715 | -3.087 | -1.953 | 1.00 | 25.59 |
| ATOM | 2444 | O | HIS | 1738 | 27.659 | -2.451 | -1.905 | 1.00 | 22.01 |
| ATOM | 2445 | N | ALA | 1739 | 29.784 | -2.651 | -2.612 | 1.00 | 23.84 |
| ATOM | 2447 | CA | ALA | 1739 | 29.759 | -1.418 | -3.388 | 1.00 | 24.93 |
| ATOM | 2448 | CB | ALA | 1739 | 31.131 | -1.177 | -4.024 | 1.00 | 26.39 |
| ATOM | 2449 | C | ALA | 1739 | 28.671 | -1.508 | -4.462 | 1.00 | 25.35 |
| ATOM | 2450 | O | ALA | 1739 | 27.963 | -0.535 | -4.727 | 1.00 | 28.20 |
| ATOM | 2451 | N | VAL | 1740 | 28.543 | -2.680 | -5.073 | 1.00 | 22.68 |
| ATOM | 2453 | CA | VAL | 1740 | 27.528 | -2.904 | -6.101 | 1.00 | 26.46 |
| ATOM | 2454 | CB | VAL | 1740 | 27.995 | -3.968 | -7.117 | 1.00 | 29.70 |
| ATOM | 2455 | CG1 | VAL | 1740 | 27.063 | -4.003 | -8.334 | 1.00 | 26.01 |
| ATOM | 2456 | CG2 | VAL | 1740 | 29.433 | -3.686 | -7.537 | 1.00 | 31.22 |
| ATOM | 2457 | C | VAL | 1740 | 26.213 | -3.358 | -5.443 | 1.00 | 25.07 |
| ATOM | 2458 | O | VAL | 1740 | 26.138 | -4.474 | -4.903 | 1.00 | 23.55 |
| ATOM | 2459 | N | PRO | 1741 | 25.155 | -2.519 | -5.514 | 1.00 | 25.30 |
| ATOM | 2460 | CD | PRO | 1741 | 25.133 | -1.190 | -6.153 | 1.00 | 22.43 |
| ATOM | 2461 | CA | PRO | 1741 | 23.844 | -2.833 | -4.921 | 1.00 | 24.09 |
| ATOM | 2462 | CB | PRO | 1741 | 22.962 | -1.675 | -5.402 | 1.00 | 23.12 |
| ATOM | 2463 | CG | PRO | 1741 | 23.928 | -0.527 | -5.491 | 1.00 | 22.04 |
| ATOM | 2464 | C | PRO | 1741 | 23.272 | -4.191 | -5.313 | 1.00 | 22.18 |
| ATOM | 2465 | O | PRO | 1741 | 22.727 | -4.900 | -4.466 | 1.00 | 21.23 |
| ATOM | 2466 | N | SER | 1742 | 23.437 | -4.570 | -6.580 | 1.00 | 23.87 |
| ATOM | 2468 | CA | SER | 1742 | 22.928 | -5.847 | -7.088 | 1.00 | 24.36 |
| ATOM | 2469 | CB | SER | 1742 | 23.071 | -5.907 | -8.612 | 1.00 | 27.39 |
| ATOM | 2470 | OG | SER | 1742 | 24.436 | -6.025 | -8.986 | 1.00 | 29.25 |
| ATOM | 2472 | C | SER | 1742 | 23.636 | -7.058 | -6.488 | 1.00 | 23.96 |
| ATOM | 2473 | O | SER | 1742 | 23.145 | -8.179 | -6.575 | 1.00 | 24.30 |
| ATOM | 2474 | N | GLN | 1743 | 24.810 | -6.839 | -5.915 | 1.00 | 24.39 |
| ATOM | 2476 | CA | GLN | 1743 | 25.558 | -7.934 | -5.345 | 1.00 | 23.15 |
| ATOM | 2477 | CB | GLN | 1743 | 27.046 | -7.755 | -5.638 | 1.00 | 23.83 |
| ATOM | 2478 | CG | GLN | 1743 | 27.359 | -7.784 | -7.126 | 1.00 | 22.84 |
| ATOM | 2479 | CD | GLN | 1743 | 26.816 | -9.036 | -7.808 | 1.00 | 24.20 |
| ATOM | 2480 | OE1 | GLN | 1743 | 27.318 | -10.135 | -7.590 | 1.00 | 21.50 |
| ATOM | 2481 | NE2 | GLN | 1743 | 25.775 | -8.871 | -8.628 | 1.00 | 22.45 |
| ATOM | 2484 | C | GLN | 1743 | 25.309 | -8.171 | -3.868 | 1.00 | 23.12 |
| ATOM | 2485 | O | GLN | 1743 | 25.816 | -9.135 | -3.317 | 1.00 | 24.96 |
| ATOM | 2486 | N | ARG | 1744 | 24.557 | -7.280 | -3.225 | 1.00 | 23.67 |
| ATOM | 2488 | CA | ARG | 1744 | 24.242 | -7.424 | -1.806 | 1.00 | 22.11 |
| ATOM | 2489 | CB | ARG | 1744 | 23.699 | -6.110 | -1.231 | 1.00 | 19.70 |
| ATOM | 2490 | CG | ARG | 1744 | 24.672 | -4.959 | -1.338 | 1.00 | 21.26 |
| ATOM | 2491 | CD | ARG | 1744 | 24.049 | -3.640 | -0.890 | 1.00 | 20.68 |
| ATOM | 2492 | NE | ARG | 1744 | 24.923 | -2.552 | -1.305 | 1.00 | 25.21 |
| ATOM | 2494 | CZ | ARG | 1744 | 24.540 | -1.313 | -1.583 | 1.00 | 24.30 |
| ATOM | 2495 | NH1 | ARG | 1744 | 23.257 | -0.955 | -1.481 | 1.00 | 22.04 |
| ATOM | 2498 | NH2 | ARG | 1744 | 25.450 | -0.448 | -2.036 | 1.00 | 21.29 |
| ATOM | 2501 | C | ARG | 1744 | 23.184 | -8.505 | -1.640 | 1.00 | 22.53 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2502 | O | ARG | 1744 | 22.437 | -8.800 | -2.588 | 1.00 | 23.08 |
| ATOM | 2503 | N | PRO | 1745 | 23.162 | -9.170 | -0.467 | 1.00 | 20.76 |
| ATOM | 2504 | CD | PRO | 1745 | 24.087 | -9.078 | 0.681 | 1.00 | 21.71 |
| ATOM | 2505 | CA | PRO | 1745 | 22.160 | -10.207 | -0.243 | 1.00 | 22.34 |
| ATOM | 2506 | CB | PRO | 1745 | 22.632 | -10.859 | 1.057 | 1.00 | 20.58 |
| ATOM | 2507 | CG | PRO | 1745 | 23.298 | -9.727 | 1.783 | 1.00 | 20.36 |
| ATOM | 2508 | C | PRO | 1745 | 20.814 | -9.512 | -0.048 | 1.00 | 23.62 |
| ATOM | 2509 | O | PRO | 1745 | 20.759 | -8.318 | 0.255 | 1.00 | 25.29 |
| ATOM | 2510 | N | THR | 1746 | 19.731 | -10.235 | -0.275 | 1.00 | 23.39 |
| ATOM | 2512 | CA | THR | 1746 | 18.404 | -9.675 | -0.080 | 1.00 | 22.77 |
| ATOM | 2513 | CB | THR | 1746 | 17.386 | -10.368 | -1.004 | 1.00 | 23.24 |
| ATOM | 2514 | OG1 | THR | 1746 | 17.409 | -11.783 | -0.763 | 1.00 | 23.11 |
| ATOM | 2516 | CG2 | THR | 1746 | 17.724 | -10.103 | -2.475 | 1.00 | 24.96 |
| ATOM | 2517 | C | THR | 1746 | 18.009 | -9.954 | 1.365 | 1.00 | 24.98 |
| ATOM | 2518 | O | THR | 1746 | 18.664 | -10.758 | 2.043 | 1.00 | 24.30 |
| ATOM | 2519 | N | PHE | 1747 | 16.944 | -9.318 | 1.853 | 1.00 | 24.95 |
| ATOM | 2521 | CA | PHE | 1747 | 16.501 | -9.596 | 3.221 | 1.00 | 25.16 |
| ATOM | 2522 | CB | PHE | 1747 | 15.395 | -8.628 | 3.661 | 1.00 | 23.64 |
| ATOM | 2523 | CG | PHE | 1747 | 15.916 | -7.283 | 4.089 | 1.00 | 24.34 |
| ATOM | 2524 | CD1 | PHE | 1747 | 16.715 | -7.167 | 5.226 | 1.00 | 21.21 |
| ATOM | 2525 | CD2 | PHE | 1747 | 15.649 | -6.137 | 3.334 | 1.00 | 21.42 |
| ATOM | 2526 | CE1 | PHE | 1747 | 17.252 | -5.932 | 5.597 | 1.00 | 20.99 |
| ATOM | 2527 | CE2 | PHE | 1747 | 16.178 | -4.907 | 3.699 | 1.00 | 20.36 |
| ATOM | 2528 | CZ | PHE | 1747 | 16.985 | -4.807 | 4.840 | 1.00 | 19.30 |
| ATOM | 2529 | C | PHE | 1747 | 16.034 | -11.049 | 3.311 | 1.00 | 23.57 |
| ATOM | 2530 | O | PHE | 1747 | 16.182 | -11.702 | 4.344 | 1.00 | 25.32 |
| ATOM | 2531 | N | LYS | 1748 | 15.520 | -11.573 | 2.202 | 1.00 | 23.19 |
| ATOM | 2533 | CA | LYS | 1748 | 15.066 | -12.958 | 2.167 | 1.00 | 23.67 |
| ATOM | 2534 | CB | LYS | 1748 | 14.462 | -13.285 | 0.799 | 1.00 | 26.67 |
| ATOM | 2535 | CG | LYS | 1748 | 14.018 | -14.739 | 0.622 | 1.00 | 30.49 |
| ATOM | 2536 | CD | LYS | 1748 | 13.642 | -14.996 | -0.837 | 1.00 | 38.98 |
| ATOM | 2537 | CE | LYS | 1748 | 13.182 | -16.432 | -1.087 | 1.00 | 44.52 |
| ATOM | 2538 | NZ | LYS | 1748 | 11.997 | -16.790 | -0.245 | 1.00 | 52.75 |
| ATOM | 2542 | C | LYS | 1748 | 16.264 | -13.865 | 2.445 | 1.00 | 25.65 |
| ATOM | 2543 | O | LYS | 1748 | 16.184 | -14.778 | 3.270 | 1.00 | 27.19 |
| ATOM | 2544 | N | GLN | 1749 | 17.378 | -13.603 | 1.762 | 1.00 | 24.56 |
| ATOM | 2546 | CA | GLN | 1749 | 18.588 | -14.397 | 1.950 | 1.00 | 26.33 |
| ATOM | 2547 | CB | GLN | 1749 | 19.702 | -13.953 | 0.993 | 1.00 | 27.97 |
| ATOM | 2548 | CG | GLN | 1749 | 19.416 | -14.066 | -0.484 | 1.00 | 37.31 |
| ATOM | 2549 | CD | GLN | 1749 | 20.518 | -13.415 | -1.315 | 1.00 | 40.24 |
| ATOM | 2550 | OE1 | GLN | 1749 | 20.296 | -12.408 | -1.970 | 1.00 | 38.83 |
| ATOM | 2551 | NE2 | GLN | 1749 | 21.726 | -13.983 | -1.259 | 1.00 | 47.83 |
| ATOM | 2554 | C | GLN | 1749 | 19.099 | -14.223 | 3.377 | 1.00 | 23.92 |
| ATOM | 2555 | O | GLN | 1749 | 19.459 | -15.196 | 4.040 | 1.00 | 25.27 |
| ATOM | 2556 | N | LEU | 1750 | 19.155 | -12.976 | 3.829 | 1.00 | 23.12 |
| ATOM | 2558 | CA | LEU | 1750 | 19.641 | -12.662 | 5.175 | 1.00 | 24.34 |
| ATOM | 2559 | CB | LEU | 1750 | 19.607 | -11.149 | 5.427 | 1.00 | 23.08 |
| ATOM | 2560 | CG | LEU | 1750 | 20.633 | -10.311 | 4.665 | 1.00 | 23.84 |
| ATOM | 2561 | CD1 | LEU | 1750 | 20.274 | -8.806 | 4.724 | 1.00 | 22.10 |
| ATOM | 2562 | CD2 | LEU | 1750 | 22.013 | -10.586 | 5.246 | 1.00 | 24.91 |
| ATOM | 2563 | C | LEU | 1750 | 18.840 | -13.400 | 6.236 | 1.00 | 27.40 |
| ATOM | 2564 | O | LEU | 1750 | 19.408 | -13.915 | 7.211 | 1.00 | 27.11 |
| ATOM | 2565 | N | VAL | 1751 | 17.527 | -13.482 | 6.031 | 1.00 | 26.83 |
| ATOM | 2567 | CA | VAL | 1751 | 16.665 | -14.174 | 6.970 | 1.00 | 25.31 |

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ATOM   2568  CB   VAL  1751   15.176  -13.994   6.599  1.00  25.87
ATOM   2569  CG1  VAL  1751   14.304  -14.975   7.382  1.00  28.43
ATOM   2570  CG2  VAL  1751   14.746  -12.593   6.934  1.00  21.52
ATOM   2571  C    VAL  1751   17.047  -15.642   7.025  1.00  25.87
ATOM   2572  O    VAL  1751   17.178  -16.218   8.106  1.00  23.41
ATOM   2573  N    GLU  1752   17.253  -16.243   5.858  1.00  29.98
ATOM   2575  CA   GLU  1752   17.631  -17.651   5.799  1.00  33.12
ATOM   2576  CB   GLU  1752   17.653  -18.134   4.346  1.00  35.99
ATOM   2577  CG   GLU  1752   16.284  -18.077   3.670  1.00  43.58
ATOM   2578  CD   GLU  1752   16.300  -18.575   2.230  1.00  48.64
ATOM   2579  OE1  GLU  1752   15.453  -18.124   1.431  1.00  48.99
ATOM   2580  OE2  GLU  1752   17.157  -19.426   1.902  1.00  55.41
ATOM   2581  C    GLU  1752   18.995  -17.891   6.467  1.00  33.15
ATOM   2582  O    GLU  1752   19.173  -18.847   7.236  1.00  30.71
ATOM   2583  N    ASP  1753   19.951  -17.011   6.186  1.00  31.12
ATOM   2585  CA   ASP  1753   21.279  -17.131   6.770  1.00  30.51
ATOM   2586  CB   ASP  1753   22.243  -16.108   6.155  1.00  29.15
ATOM   2587  CG   ASP  1753   22.488  -16.344   4.672  1.00  33.53
ATOM   2588  OD1  ASP  1753   22.361  -17.494   4.215  1.00  34.92
ATOM   2589  OD2  ASP  1753   22.815  -15.371   3.955  1.00  38.26
ATOM   2590  C    ASP  1753   21.215  -16.968   8.287  1.00  28.54
ATOM   2591  O    ASP  1753   21.739  -17.800   9.025  1.00  28.95
ATOM   2592  N    LEU  1754   20.537  -15.926   8.753  1.00  27.25
ATOM   2594  CA   LEU  1754   20.421  -15.673  10.193  1.00  28.08
ATOM   2595  CB   LEU  1754   19.754  -14.328  10.455  1.00  23.31
ATOM   2596  CG   LEU  1754   20.733  -13.199  10.160  1.00  24.47
ATOM   2597  CD1  LEU  1754   20.007  -11.863  10.094  1.00  19.58
ATOM   2598  CD2  LEU  1754   21.846  -13.207  11.216  1.00  21.17
ATOM   2599  C    LEU  1754   19.688  -16.789  10.921  1.00  31.61
ATOM   2600  O    LEU  1754   20.037  -17.135  12.048  1.00  32.64
ATOM   2601  N    ASP  1755   18.690  -17.367  10.259  1.00  32.61
ATOM   2603  CA   ASP  1755   17.931  -18.460  10.833  1.00  34.20
ATOM   2604  CB   ASP  1755   16.823  -18.883   9.872  1.00  37.70
ATOM   2605  CG   ASP  1755   15.808  -19.780  10.526  1.00  44.27
ATOM   2606  OD1  ASP  1755   15.445  -19.521  11.692  1.00  47.16
ATOM   2607  OD2  ASP  1755   15.370  -20.745   9.876  1.00  51.35
ATOM   2608  C    ASP  1755   18.894  -19.616  11.073  1.00  34.63
ATOM   2609  O    ASP  1755   18.858  -20.273  12.119  1.00  36.24
ATOM   2610  N    ARG  1756   19.782  -19.826  10.108  1.00  32.60
ATOM   2612  CA   ARG  1756   20.784  -20.870  10.190  1.00  33.69
ATOM   2613  CB   ARG  1756   21.548  -20.939   8.867  1.00  35.42
ATOM   2614  CG   ARG  1756   22.639  -22.003   8.800  1.00  40.87
ATOM   2615  CD   ARG  1756   23.212  -22.094   7.395  1.00  42.73
ATOM   2616  NE   ARG  1756   23.739  -20.813   6.926  1.00  48.45
ATOM   2618  CZ   ARG  1756   24.882  -20.274   7.340  1.00  49.90
ATOM   2619  NH1  ARG  1756   25.634  -20.905   8.243  1.00  49.63
ATOM   2622  NH2  ARG  1756   25.276  -19.105   6.844  1.00  50.86
ATOM   2625  C    ARG  1756   21.748  -20.598  11.345  1.00  34.78
ATOM   2626  O    ARG  1756   21.929  -21.436  12.228  1.00  36.24
ATOM   2627  N    ILE  1757   22.325  -19.402  11.363  1.00  35.35
ATOM   2629  CA   ILE  1757   23.281  -19.018  12.392  1.00  35.54
ATOM   2630  CB   ILE  1757   23.905  -17.631  12.103  1.00  34.99
ATOM   2631  CG2  ILE  1757   24.955  -17.303  13.159  1.00  32.06
ATOM   2632  CG1  ILE  1757   24.547  -17.626  10.711  1.00  33.77
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2633 | CD1 | ILE | 1757 | 24.908 | -16.247 | 10.185 | 1.00 | 31.44 |
| ATOM | 2634 | C | ILE | 1757 | 22.698 | -19.036 | 13.803 | 1.00 | 36.49 |
| ATOM | 2635 | O | ILE | 1757 | 23.337 | -19.548 | 14.716 | 1.00 | 36.40 |
| ATOM | 2636 | N | VAL | 1758 | 21.487 | -18.515 | 13.988 | 1.00 | 36.91 |
| ATOM | 2638 | CA | VAL | 1758 | 20.881 | -18.498 | 15.322 | 1.00 | 38.68 |
| ATOM | 2639 | CB | VAL | 1758 | 19.425 | -17.962 | 15.312 | 1.00 | 37.77 |
| ATOM | 2640 | CG1 | VAL | 1758 | 18.806 | -18.059 | 16.708 | 1.00 | 38.39 |
| ATOM | 2641 | CG2 | VAL | 1758 | 19.392 | -16.524 | 14.854 | 1.00 | 36.69 |
| ATOM | 2642 | C | VAL | 1758 | 20.891 | -19.908 | 15.895 | 1.00 | 41.38 |
| ATOM | 2643 | O | VAL | 1758 | 21.405 | -20.138 | 16.997 | 1.00 | 42.41 |
| ATOM | 2644 | N | ALA | 1759 | 20.379 | -20.851 | 15.111 | 1.00 | 40.59 |
| ATOM | 2646 | CA | ALA | 1759 | 20.325 | -22.247 | 15.508 | 1.00 | 40.84 |
| ATOM | 2647 | CB | ALA | 1759 | 19.741 | -23.074 | 14.384 | 1.00 | 40.20 |
| ATOM | 2648 | C | ALA | 1759 | 21.703 | -22.787 | 15.897 | 1.00 | 42.52 |
| ATOM | 2649 | O | ALA | 1759 | 21.822 | -23.594 | 16.809 | 1.00 | 44.78 |
| ATOM | 2650 | N | LEU | 1760 | 22.740 | -22.339 | 15.208 | 1.00 | 43.16 |
| ATOM | 2652 | CA | LEU | 1760 | 24.095 | -22.800 | 15.493 | 1.00 | 46.98 |
| ATOM | 2653 | CB | LEU | 1760 | 24.921 | -22.761 | 14.203 | 1.00 | 47.66 |
| ATOM | 2654 | CG | LEU | 1760 | 24.286 | -23.545 | 13.060 | 1.00 | 52.77 |
| ATOM | 2655 | CD1 | LEU | 1760 | 24.973 | -23.222 | 11.745 | 1.00 | 56.58 |
| ATOM | 2656 | CD2 | LEU | 1760 | 24.343 | -25.038 | 13.369 | 1.00 | 53.06 |
| ATOM | 2657 | C | LEU | 1760 | 24.811 | -21.986 | 16.573 | 1.00 | 47.43 |
| ATOM | 2658 | O | LEU | 1760 | 25.917 | -22.335 | 16.989 | 1.00 | 46.58 |
| ATOM | 2659 | N | THR | 1761 | 24.183 | -20.914 | 17.034 | 1.00 | 48.65 |
| ATOM | 2661 | CA | THR | 1761 | 24.814 | -20.055 | 18.021 | 1.00 | 49.69 |
| ATOM | 2662 | CB | THR | 1761 | 24.382 | -18.570 | 17.831 | 1.00 | 50.15 |
| ATOM | 2663 | OG1 | THR | 1761 | 24.783 | -18.127 | 16.529 | 1.00 | 49.87 |
| ATOM | 2665 | CG2 | THR | 1761 | 25.063 | -17.671 | 18.843 | 1.00 | 48.64 |
| ATOM | 2666 | C | THR | 1761 | 24.673 | -20.497 | 19.475 | 1.00 | 50.33 |
| ATOM | 2667 | O | THR | 1761 | 23.584 | -20.825 | 19.947 | 1.00 | 48.81 |
| ATOM | 2668 | N | SER | 1762 | 25.811 | -20.511 | 20.166 | 1.00 | 50.25 |
| ATOM | 2670 | CA | SER | 1762 | 25.891 | -20.890 | 21.566 | 1.00 | 50.98 |
| ATOM | 2671 | CB | SER | 1762 | 27.362 | -20.887 | 22.002 | 1.00 | 54.71 |
| ATOM | 2672 | OG | SER | 1762 | 27.537 | -21.423 | 23.308 | 1.00 | 57.99 |
| ATOM | 2674 | C | SER | 1762 | 25.083 | -19.914 | 22.425 | 1.00 | 49.39 |
| ATOM | 2675 | O | SER | 1762 | 25.297 | -18.694 | 22.370 | 1.00 | 48.00 |
| ATOM | 3474 | N | SER | 461 | 79.623 | 25.766 | 14.533 | 1.00 | 48.84 |
| ATOM | 3476 | CA | SER | 461 | 79.566 | 24.645 | 13.593 | 1.00 | 46.93 |
| ATOM | 3477 | CB | SER | 461 | 78.276 | 23.838 | 13.809 | 1.00 | 46.66 |
| ATOM | 3478 | C | SER | 461 | 79.676 | 25.114 | 12.138 | 1.00 | 43.02 |
| ATOM | 3479 | O | SER | 461 | 79.692 | 24.301 | 11.210 | 1.00 | 40.19 |
| ATOM | 3480 | N | GLU | 462 | 79.791 | 26.427 | 11.956 | 1.00 | 41.48 |
| ATOM | 3482 | CA | GLU | 462 | 79.904 | 27.034 | 10.628 | 1.00 | 39.59 |
| ATOM | 3483 | CB | GLU | 462 | 80.021 | 28.560 | 10.744 | 1.00 | 40.66 |
| ATOM | 3484 | C | GLU | 462 | 81.054 | 26.480 | 9.796 | 1.00 | 36.60 |
| ATOM | 3485 | O | GLU | 462 | 80.852 | 26.121 | 8.641 | 1.00 | 35.10 |
| ATOM | 3486 | N | TYR | 463 | 82.252 | 26.416 | 10.380 | 1.00 | 36.07 |
| ATOM | 3488 | CA | TYR | 463 | 83.430 | 25.916 | 9.673 | 1.00 | 35.60 |
| ATOM | 3489 | CB | TYR | 463 | 84.597 | 26.906 | 9.755 | 1.00 | 38.15 |
| ATOM | 3490 | CG | TYR | 463 | 84.372 | 28.104 | 8.861 | 1.00 | 44.08 |
| ATOM | 3491 | CD1 | TYR | 463 | 84.137 | 29.368 | 9.406 | 1.00 | 44.99 |
| ATOM | 3492 | CE1 | TYR | 463 | 83.833 | 30.451 | 8.593 | 1.00 | 46.88 |
| ATOM | 3493 | CD2 | TYR | 463 | 84.305 | 27.959 | 7.464 | 1.00 | 43.95 |
| ATOM | 3494 | CE2 | TYR | 463 | 84.003 | 29.044 | 6.642 | 1.00 | 41.86 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3495 | CZ | TYR | 463 | 83.768 | 30.282 | 7.215 | 1.00 | 43.89 |
| ATOM | 3496 | OH | TYR | 463 | 83.468 | 31.364 | 6.431 | 1.00 | 44.37 |
| ATOM | 3498 | C | TYR | 463 | 83.903 | 24.520 | 10.014 | 1.00 | 33.90 |
| ATOM | 3499 | O | TYR | 463 | 84.440 | 23.828 | 9.147 | 1.00 | 33.90 |
| ATOM | 3500 | N | GLU | 464 | 83.742 | 24.098 | 11.260 | 1.00 | 32.81 |
| ATOM | 3502 | CA | GLU | 464 | 84.167 | 22.753 | 11.633 | 1.00 | 34.64 |
| ATOM | 3503 | CB | GLU | 464 | 85.663 | 22.727 | 11.919 | 1.00 | 37.48 |
| ATOM | 3504 | CG | GLU | 464 | 86.075 | 23.633 | 13.049 | 1.00 | 45.48 |
| ATOM | 3505 | CD | GLU | 464 | 87.552 | 23.987 | 13.015 | 1.00 | 55.80 |
| ATOM | 3506 | OE1 | GLU | 464 | 87.920 | 24.996 | 13.659 | 1.00 | 61.78 |
| ATOM | 3507 | OE2 | GLU | 464 | 88.344 | 23.271 | 12.351 | 1.00 | 58.34 |
| ATOM | 3508 | C | GLU | 464 | 83.426 | 22.296 | 12.858 | 1.00 | 33.05 |
| ATOM | 3509 | O | GLU | 464 | 83.083 | 23.119 | 13.705 | 1.00 | 34.54 |
| ATOM | 3510 | N | LEU | 465 | 83.147 | 21.001 | 12.943 | 1.00 | 32.59 |
| ATOM | 3512 | CA | LEU | 465 | 82.462 | 20.463 | 14.114 | 1.00 | 33.74 |
| ATOM | 3513 | CB | LEU | 465 | 81.484 | 19.341 | 13.747 | 1.00 | 31.20 |
| ATOM | 3514 | CG | LEU | 465 | 80.510 | 19.433 | 12.577 | 1.00 | 32.77 |
| ATOM | 3515 | CD1 | LEU | 465 | 79.355 | 18.492 | 12.858 | 1.00 | 26.22 |
| ATOM | 3516 | CD2 | LEU | 465 | 80.021 | 20.846 | 12.359 | 1.00 | 31.59 |
| ATOM | 3517 | C | LEU | 465 | 83.511 | 19.889 | 15.059 | 1.00 | 35.64 |
| ATOM | 3518 | O | LEU | 465 | 84.641 | 19.574 | 14.642 | 1.00 | 33.77 |
| ATOM | 3519 | N | PRO | 466 | 83.150 | 19.734 | 16.349 | 1.00 | 36.71 |
| ATOM | 3520 | CD | PRO | 466 | 81.865 | 20.104 | 16.967 | 1.00 | 36.97 |
| ATOM | 3521 | CA | PRO | 466 | 84.074 | 19.185 | 17.346 | 1.00 | 36.17 |
| ATOM | 3522 | CB | PRO | 466 | 83.247 | 19.196 | 18.626 | 1.00 | 36.83 |
| ATOM | 3523 | CG | PRO | 466 | 82.274 | 20.326 | 18.394 | 1.00 | 40.80 |
| ATOM | 3524 | C | PRO | 466 | 84.419 | 17.765 | 16.950 | 1.00 | 37.39 |
| ATOM | 3525 | O | PRO | 466 | 83.626 | 17.077 | 16.297 | 1.00 | 34.71 |
| ATOM | 3526 | N | GLU | 467 | 85.611 | 17.330 | 17.315 | 1.00 | 38.40 |
| ATOM | 3528 | CA | GLU | 467 | 86.030 | 15.987 | 16.976 | 1.00 | 42.59 |
| ATOM | 3529 | CB | GLU | 467 | 87.493 | 15.987 | 16.540 | 1.00 | 49.21 |
| ATOM | 3530 | CG | GLU | 467 | 87.922 | 14.682 | 15.891 | 1.00 | 58.93 |
| ATOM | 3531 | CD | GLU | 467 | 89.276 | 14.769 | 15.213 | 1.00 | 64.76 |
| ATOM | 3532 | OE1 | GLU | 467 | 90.013 | 15.767 | 15.426 | 1.00 | 63.57 |
| ATOM | 3533 | OE2 | GLU | 467 | 89.592 | 13.823 | 14.458 | 1.00 | 69.03 |
| ATOM | 3534 | C | GLU | 467 | 85.825 | 15.037 | 18.146 | 1.00 | 40.74 |
| ATOM | 3535 | O | GLU | 467 | 85.938 | 15.430 | 19.309 | 1.00 | 41.52 |
| ATOM | 3536 | N | ASP | 468 | 85.472 | 13.802 | 17.831 | 1.00 | 38.57 |
| ATOM | 3538 | CA | ASP | 468 | 85.273 | 12.776 | 18.851 | 1.00 | 40.86 |
| ATOM | 3539 | CB | ASP | 468 | 83.793 | 12.640 | 19.224 | 1.00 | 40.27 |
| ATOM | 3540 | CG | ASP | 468 | 83.566 | 11.697 | 20.397 | 1.00 | 41.36 |
| ATOM | 3541 | OD1 | ASP | 468 | 82.429 | 11.670 | 20.919 | 1.00 | 42.50 |
| ATOM | 3542 | OD2 | ASP | 468 | 84.514 | 10.992 | 20.807 | 1.00 | 38.55 |
| ATOM | 3543 | C | ASP | 468 | 85.803 | 11.470 | 18.278 | 1.00 | 40.75 |
| ATOM | 3544 | O | ASP | 468 | 85.068 | 10.701 | 17.650 | 1.00 | 41.80 |
| ATOM | 3545 | N | PRO | 469 | 87.100 | 11.209 | 18.481 | 1.00 | 41.71 |
| ATOM | 3546 | CD | PRO | 469 | 88.001 | 12.062 | 19.276 | 1.00 | 41.87 |
| ATOM | 3547 | CA | PRO | 469 | 87.801 | 10.011 | 18.012 | 1.00 | 40.07 |
| ATOM | 3548 | CB | PRO | 469 | 89.091 | 10.042 | 18.831 | 1.00 | 40.42 |
| ATOM | 3549 | CG | PRO | 469 | 89.366 | 11.505 | 18.938 | 1.00 | 39.42 |
| ATOM | 3550 | C | PRO | 469 | 87.033 | 8.720 | 18.260 | 1.00 | 41.00 |
| ATOM | 3551 | O | PRO | 469 | 87.032 | 7.822 | 17.414 | 1.00 | 41.75 |
| ATOM | 3552 | N | ARG | 470 | 86.361 | 8.639 | 19.411 | 1.00 | 40.70 |
| ATOM | 3554 | CA | ARG | 470 | 85.600 | 7.446 | 19.779 | 1.00 | 41.03 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3555 | CB | ARG | 470 | 84.827 | 7.677 | 21.075 | 1.00 | 44.18 |
| ATOM | 3556 | CG | ARG | 470 | 85.628 | 8.240 | 22.218 | 1.00 | 47.89 |
| ATOM | 3557 | CD | ARG | 470 | 84.719 | 8.518 | 23.400 | 1.00 | 50.56 |
| ATOM | 3558 | NE | ARG | 470 | 83.576 | 9.345 | 23.023 | 1.00 | 51.20 |
| ATOM | 3560 | CZ | ARG | 470 | 82.695 | 9.845 | 23.881 | 1.00 | 52.24 |
| ATOM | 3561 | NH1 | ARG | 470 | 82.818 | 9.608 | 25.183 | 1.00 | 51.31 |
| ATOM | 3564 | NH2 | ARG | 470 | 81.672 | 10.564 | 23.432 | 1.00 | 52.73 |
| ATOM | 3567 | C | ARG | 470 | 84.596 | 7.004 | 18.723 | 1.00 | 39.03 |
| ATOM | 3568 | O | ARG | 470 | 84.401 | 5.813 | 18.518 | 1.00 | 40.72 |
| ATOM | 3569 | N | TRP | 471 | 83.972 | 7.965 | 18.050 | 1.00 | 37.77 |
| ATOM | 3571 | CA | TRP | 471 | 82.948 | 7.656 | 17.059 | 1.00 | 36.73 |
| ATOM | 3572 | CB | TRP | 471 | 81.672 | 8.401 | 17.432 | 1.00 | 35.05 |
| ATOM | 3573 | CG | TRP | 471 | 81.044 | 7.862 | 18.673 | 1.00 | 34.85 |
| ATOM | 3574 | CD2 | TRP | 471 | 80.235 | 6.687 | 18.766 | 1.00 | 34.96 |
| ATOM | 3575 | CE2 | TRP | 471 | 79.831 | 6.564 | 20.116 | 1.00 | 35.12 |
| ATOM | 3576 | CE3 | TRP | 471 | 79.810 | 5.721 | 17.838 | 1.00 | 33.25 |
| ATOM | 3577 | CD1 | TRP | 471 | 81.106 | 8.390 | 19.933 | 1.00 | 29.97 |
| ATOM | 3578 | NE1 | TRP | 471 | 80.377 | 7.616 | 20.805 | 1.00 | 32.18 |
| ATOM | 3580 | CZ2 | TRP | 471 | 79.017 | 5.512 | 20.560 | 1.00 | 33.98 |
| ATOM | 3581 | CZ3 | TRP | 471 | 79.002 | 4.673 | 18.282 | 1.00 | 33.71 |
| ATOM | 3582 | CH2 | TRP | 471 | 78.618 | 4.580 | 19.632 | 1.00 | 33.28 |
| ATOM | 3583 | C | TRP | 471 | 83.275 | 7.930 | 15.599 | 1.00 | 37.27 |
| ATOM | 3584 | O | TRP | 471 | 82.580 | 7.445 | 14.695 | 1.00 | 36.61 |
| ATOM | 3585 | N | GLU | 472 | 84.341 | 8.680 | 15.361 | 1.00 | 37.93 |
| ATOM | 3587 | CA | GLU | 472 | 84.706 | 9.054 | 14.004 | 1.00 | 37.08 |
| ATOM | 3588 | CB | GLU | 472 | 85.865 | 10.049 | 14.045 | 1.00 | 36.30 |
| ATOM | 3589 | CG | GLU | 472 | 86.026 | 10.851 | 12.773 | 1.00 | 33.51 |
| ATOM | 3590 | CD | GLU | 472 | 84.931 | 11.895 | 12.580 | 1.00 | 33.80 |
| ATOM | 3591 | OE1 | GLU | 472 | 84.385 | 12.408 | 13.581 | 1.00 | 35.19 |
| ATOM | 3592 | OE2 | GLU | 472 | 84.641 | 12.226 | 11.412 | 1.00 | 32.51 |
| ATOM | 3593 | C | GLU | 472 | 85.021 | 7.923 | 13.032 | 1.00 | 37.88 |
| ATOM | 3594 | O | GLU | 472 | 85.774 | 7.000 | 13.351 | 1.00 | 38.20 |
| ATOM | 3595 | N | LEU | 473 | 84.422 | 7.992 | 11.846 | 1.00 | 37.55 |
| ATOM | 3597 | CA | LEU | 473 | 84.678 | 7.004 | 10.813 | 1.00 | 36.93 |
| ATOM | 3598 | CB | LEU | 473 | 83.404 | 6.244 | 10.443 | 1.00 | 37.08 |
| ATOM | 3599 | CG | LEU | 473 | 83.680 | 5.086 | 9.470 | 1.00 | 39.14 |
| ATOM | 3600 | CD1 | LEU | 473 | 84.196 | 3.877 | 10.250 | 1.00 | 38.39 |
| ATOM | 3601 | CD2 | LEU | 473 | 82.433 | 4.716 | 8.672 | 1.00 | 39.46 |
| ATOM | 3602 | C | LEU | 473 | 85.207 | 7.732 | 9.577 | 1.00 | 38.52 |
| ATOM | 3603 | O | LEU | 473 | 84.660 | 8.764 | 9.182 | 1.00 | 38.67 |
| ATOM | 3604 | N | PRO | 474 | 86.334 | 7.259 | 9.005 | 1.00 | 39.02 |
| ATOM | 3605 | CD | PRO | 474 | 87.259 | 6.259 | 9.571 | 1.00 | 38.39 |
| ATOM | 3606 | CA | PRO | 474 | 86.918 | 7.877 | 7.809 | 1.00 | 38.24 |
| ATOM | 3607 | CB | PRO | 474 | 88.188 | 7.049 | 7.590 | 1.00 | 38.40 |
| ATOM | 3608 | CG | PRO | 474 | 88.580 | 6.680 | 8.979 | 1.00 | 35.50 |
| ATOM | 3609 | C | PRO | 474 | 85.942 | 7.727 | 6.642 | 1.00 | 37.56 |
| ATOM | 3610 | O | PRO | 474 | 85.415 | 6.641 | 6.400 | 1.00 | 37.88 |
| ATOM | 3611 | N | ARG | 475 | 85.720 | 8.809 | 5.907 | 1.00 | 37.73 |
| ATOM | 3613 | CA | ARG | 475 | 84.779 | 8.790 | 4.795 | 1.00 | 40.01 |
| ATOM | 3614 | CB | ARG | 475 | 84.655 | 10.183 | 4.182 | 1.00 | 38.31 |
| ATOM | 3615 | CG | ARG | 475 | 84.217 | 11.236 | 5.198 | 1.00 | 35.15 |
| ATOM | 3616 | CD | ARG | 475 | 84.069 | 12.631 | 4.586 | 1.00 | 33.92 |
| ATOM | 3617 | NE | ARG | 475 | 83.718 | 13.603 | 5.616 | 1.00 | 30.45 |
| ATOM | 3619 | CZ | ARG | 475 | 82.475 | 13.880 | 5.993 | 1.00 | 26.48 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3620 | NH1 | ARG | 475 | 81.444 | 13.284 | 5.407 | 1.00 | 24.80 |
| ATOM | 3623 | NH2 | ARG | 475 | 82.271 | 14.650 | 7.056 | 1.00 | 25.16 |
| ATOM | 3626 | C | ARG | 475 | 85.054 | 7.735 | 3.728 | 1.00 | 42.18 |
| ATOM | 3627 | O | ARG | 475 | 84.125 | 7.197 | 3.128 | 1.00 | 41.43 |
| ATOM | 3628 | N | ASP | 476 | 86.322 | 7.391 | 3.535 | 1.00 | 45.44 |
| ATOM | 3630 | CA | ASP | 476 | 86.676 | 6.387 | 2.541 | 1.00 | 49.80 |
| ATOM | 3631 | CB | ASP | 476 | 88.192 | 6.343 | 2.329 | 1.00 | 50.95 |
| ATOM | 3632 | CG | ASP | 476 | 88.944 | 5.975 | 3.585 | 1.00 | 53.89 |
| ATOM | 3633 | OD1 | ASP | 476 | 89.303 | 4.789 | 3.731 | 1.00 | 59.71 |
| ATOM | 3634 | OD2 | ASP | 476 | 89.176 | 6.867 | 4.427 | 1.00 | 57.39 |
| ATOM | 3635 | C | ASP | 476 | 86.149 | 5.010 | 2.950 | 1.00 | 51.23 |
| ATOM | 3636 | O | ASP | 476 | 86.051 | 4.102 | 2.121 | 1.00 | 53.54 |
| ATOM | 3637 | N | ARG | 477 | 85.814 | 4.864 | 4.230 | 1.00 | 50.49 |
| ATOM | 3639 | CA | ARG | 477 | 85.285 | 3.610 | 4.753 | 1.00 | 49.32 |
| ATOM | 3640 | CB | ARG | 477 | 85.834 | 3.364 | 6.152 | 1.00 | 49.79 |
| ATOM | 3641 | CG | ARG | 477 | 87.237 | 2.806 | 6.112 | 1.00 | 53.06 |
| ATOM | 3642 | CD | ARG | 477 | 87.960 | 2.981 | 7.420 | 1.00 | 56.76 |
| ATOM | 3643 | NE | ARG | 477 | 87.310 | 2.293 | 8.529 | 1.00 | 59.35 |
| ATOM | 3645 | CZ | ARG | 477 | 87.728 | 2.371 | 9.789 | 1.00 | 62.23 |
| ATOM | 3646 | NH1 | ARG | 477 | 88.793 | 3.103 | 10.101 | 1.00 | 63.66 |
| ATOM | 3649 | NH2 | ARG | 477 | 87.067 | 1.741 | 10.745 | 1.00 | 64.35 |
| ATOM | 3652 | C | ARG | 477 | 83.755 | 3.547 | 4.750 | 1.00 | 48.04 |
| ATOM | 3653 | O | ARG | 477 | 83.160 | 2.693 | 5.404 | 1.00 | 48.09 |
| ATOM | 3654 | N | LEU | 478 | 83.129 | 4.412 | 3.958 | 1.00 | 45.38 |
| ATOM | 3656 | CA | LEU | 478 | 81.685 | 4.469 | 3.870 | 1.00 | 41.60 |
| ATOM | 3657 | CB | LEU | 478 | 81.168 | 5.578 | 4.790 | 1.00 | 38.39 |
| ATOM | 3658 | CG | LEU | 478 | 79.651 | 5.699 | 4.894 | 1.00 | 36.38 |
| ATOM | 3659 | CD1 | LEU | 478 | 79.113 | 4.595 | 5.802 | 1.00 | 33.98 |
| ATOM | 3660 | CD2 | LEU | 478 | 79.293 | 7.068 | 5.441 | 1.00 | 40.06 |
| ATOM | 3661 | C | LEU | 478 | 81.279 | 4.774 | 2.433 | 1.00 | 41.92 |
| ATOM | 3662 | O | LEU | 478 | 81.696 | 5.780 | 1.870 | 1.00 | 43.99 |
| ATOM | 3663 | N | VAL | 479 | 80.466 | 3.904 | 1.844 | 1.00 | 42.29 |
| ATOM | 3665 | CA | VAL | 479 | 79.992 | 4.082 | 0.471 | 1.00 | 41.07 |
| ATOM | 3666 | CB | VAL | 479 | 80.227 | 2.816 | -0.397 | 1.00 | 41.13 |
| ATOM | 3667 | CG1 | VAL | 479 | 79.719 | 3.057 | -1.810 | 1.00 | 40.19 |
| ATOM | 3668 | CG2 | VAL | 479 | 81.700 | 2.448 | -0.420 | 1.00 | 41.36 |
| ATOM | 3669 | C | VAL | 479 | 78.500 | 4.345 | 0.540 | 1.00 | 40.44 |
| ATOM | 3670 | O | VAL | 479 | 77.719 | 3.451 | 0.885 | 1.00 | 39.86 |
| ATOM | 3671 | N | LEU | 480 | 78.112 | 5.582 | 0.253 | 1.00 | 41.37 |
| ATOM | 3673 | CA | LEU | 480 | 76.706 | 5.973 | 0.293 | 1.00 | 41.63 |
| ATOM | 3674 | CB | LEU | 480 | 76.568 | 7.492 | 0.166 | 1.00 | 39.91 |
| ATOM | 3675 | CG | LEU | 480 | 77.236 | 8.332 | 1.261 | 1.00 | 39.23 |
| ATOM | 3676 | CD1 | LEU | 480 | 76.890 | 9.800 | 1.039 | 1.00 | 37.73 |
| ATOM | 3677 | CD2 | LEU | 480 | 76.791 | 7.877 | 2.647 | 1.00 | 35.18 |
| ATOM | 3678 | C | LEU | 480 | 75.899 | 5.273 | -0.788 | 1.00 | 42.21 |
| ATOM | 3679 | O | LEU | 480 | 76.395 | 5.048 | -1.890 | 1.00 | 45.27 |
| ATOM | 3680 | N | GLY | 481 | 74.650 | 4.947 | -0.476 | 1.00 | 41.51 |
| ATOM | 3682 | CA | GLY | 481 | 73.812 | 4.257 | -1.433 | 1.00 | 40.19 |
| ATOM | 3683 | C | GLY | 481 | 72.446 | 4.872 | -1.640 | 1.00 | 41.58 |
| ATOM | 3684 | O | GLY | 481 | 72.262 | 6.091 | -1.550 | 1.00 | 41.35 |
| ATOM | 3685 | N | LYS | 482 | 71.474 | 4.009 | -1.908 | 1.00 | 42.65 |
| ATOM | 3687 | CA | LYS | 482 | 70.105 | 4.429 | -2.166 | 1.00 | 44.17 |
| ATOM | 3688 | CB | LYS | 482 | 69.240 | 3.221 | -2.542 | 1.00 | 45.66 |
| ATOM | 3689 | C | LYS | 482 | 69.475 | 5.148 | -0.994 | 1.00 | 44.86 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3690 | O | LYS | 482 | 69.638 | 4.752 | 0.155 | 1.00 | 45.23 |
| ATOM | 3691 | N | PRO | 483 | 68.749 | 6.234 | -1.273 | 1.00 | 45.94 |
| ATOM | 3692 | CD | PRO | 483 | 68.518 | 6.880 | -2.576 | 1.00 | 46.96 |
| ATOM | 3693 | CA | PRO | 483 | 68.099 | 6.983 | -0.206 | 1.00 | 47.79 |
| ATOM | 3694 | CB | PRO | 483 | 67.542 | 8.200 | -0.947 | 1.00 | 47.02 |
| ATOM | 3695 | CG | PRO | 483 | 67.269 | 7.666 | -2.307 | 1.00 | 46.65 |
| ATOM | 3696 | C | PRO | 483 | 66.991 | 6.151 | 0.429 | 1.00 | 48.74 |
| ATOM | 3697 | O | PRO | 483 | 66.314 | 5.376 | -0.251 | 1.00 | 48.01 |
| ATOM | 3698 | N | LEU | 484 | 66.858 | 6.268 | 1.742 | 1.00 | 49.91 |
| ATOM | 3700 | CA | LEU | 484 | 65.837 | 5.547 | 2.477 | 1.00 | 53.93 |
| ATOM | 3701 | CB | LEU | 484 | 66.433 | 4.883 | 3.720 | 1.00 | 50.17 |
| ATOM | 3702 | CG | LEU | 484 | 67.517 | 3.844 | 3.445 | 1.00 | 48.93 |
| ATOM | 3703 | CD1 | LEU | 484 | 68.226 | 3.460 | 4.731 | 1.00 | 49.05 |
| ATOM | 3704 | CD2 | LEU | 484 | 66.906 | 2.630 | 2.784 | 1.00 | 47.03 |
| ATOM | 3705 | C | LEU | 484 | 64.715 | 6.501 | 2.878 | 1.00 | 58.70 |
| ATOM | 3706 | O | LEU | 484 | 63.571 | 6.075 | 3.055 | 1.00 | 61.95 |
| ATOM | 3707 | N | GLY | 485 | 65.027 | 7.788 | 3.006 | 1.00 | 60.35 |
| ATOM | 3709 | CA | GLY | 485 | 63.998 | 8.737 | 3.397 | 1.00 | 64.00 |
| ATOM | 3710 | C | GLY | 485 | 64.445 | 10.183 | 3.476 | 1.00 | 66.09 |
| ATOM | 3711 | O | GLY | 485 | 65.643 | 10.468 | 3.577 | 1.00 | 65.26 |
| ATOM | 3712 | N | GLU | 486 | 63.471 | 11.090 | 3.458 | 1.00 | 67.18 |
| ATOM | 3714 | CA | GLU | 486 | 63.733 | 12.525 | 3.508 | 1.00 | 68.69 |
| ATOM | 3715 | CB | GLU | 486 | 63.873 | 13.084 | 2.091 | 1.00 | 69.88 |
| ATOM | 3716 | C | GLU | 486 | 62.618 | 13.249 | 4.245 | 1.00 | 68.80 |
| ATOM | 3717 | O | GLU | 486 | 61.481 | 12.775 | 4.295 | 1.00 | 69.26 |
| ATOM | 3718 | N | GLY | 487 | 62.943 | 14.415 | 4.791 | 1.00 | 68.47 |
| ATOM | 3720 | CA | GLY | 487 | 61.960 | 15.188 | 5.520 | 1.00 | 67.56 |
| ATOM | 3721 | C | GLY | 487 | 62.373 | 16.635 | 5.634 | 1.00 | 66.71 |
| ATOM | 3722 | O | GLY | 487 | 63.040 | 17.172 | 4.747 | 1.00 | 66.48 |
| ATOM | 3723 | N | ALA | 488 | 61.979 | 17.265 | 6.735 | 1.00 | 67.22 |
| ATOM | 3725 | CA | ALA | 488 | 62.304 | 18.661 | 6.992 | 1.00 | 67.78 |
| ATOM | 3726 | CB | ALA | 488 | 61.637 | 19.121 | 8.283 | 1.00 | 68.97 |
| ATOM | 3727 | C | ALA | 488 | 63.817 | 18.830 | 7.085 | 1.00 | 67.38 |
| ATOM | 3728 | O | ALA | 488 | 64.413 | 18.597 | 8.141 | 1.00 | 67.14 |
| ATOM | 3729 | N | PHE | 489 | 64.429 | 19.155 | 5.946 | 1.00 | 66.22 |
| ATOM | 3731 | CA | PHE | 489 | 65.877 | 19.364 | 5.831 | 1.00 | 65.49 |
| ATOM | 3732 | CB | PHE | 489 | 66.277 | 20.699 | 6.467 | 1.00 | 66.11 |
| ATOM | 3733 | C | PHE | 489 | 66.749 | 18.207 | 6.368 | 1.00 | 64.07 |
| ATOM | 3734 | O | PHE | 489 | 67.924 | 18.399 | 6.731 | 1.00 | 61.56 |
| ATOM | 3735 | N | GLY | 490 | 66.171 | 17.005 | 6.349 | 1.00 | 60.79 |
| ATOM | 3737 | CA | GLY | 490 | 66.852 | 15.803 | 6.797 | 1.00 | 54.72 |
| ATOM | 3738 | C | GLY | 490 | 66.787 | 14.760 | 5.692 | 1.00 | 51.78 |
| ATOM | 3739 | O | GLY | 490 | 65.765 | 14.624 | 5.013 | 1.00 | 49.17 |
| ATOM | 3740 | N | GLN | 491 | 67.874 | 14.015 | 5.528 | 1.00 | 49.97 |
| ATOM | 3742 | CA | GLN | 491 | 68.000 | 12.984 | 4.504 | 1.00 | 48.06 |
| ATOM | 3743 | CB | GLN | 491 | 68.891 | 13.520 | 3.371 | 1.00 | 51.02 |
| ATOM | 3744 | CG | GLN | 491 | 69.286 | 12.518 | 2.289 | 1.00 | 56.00 |
| ATOM | 3745 | CD | GLN | 491 | 70.155 | 13.143 | 1.202 | 1.00 | 58.93 |
| ATOM | 3746 | OE1 | GLN | 491 | 70.483 | 14.330 | 1.255 | 1.00 | 60.31 |
| ATOM | 3747 | NE2 | GLN | 491 | 70.529 | 12.341 | 0.202 | 1.00 | 60.19 |
| ATOM | 3750 | C | GLN | 491 | 68.623 | 11.720 | 5.114 | 1.00 | 45.59 |
| ATOM | 3751 | O | GLN | 491 | 69.511 | 11.792 | 5.959 | 1.00 | 45.22 |
| ATOM | 3752 | N | VAL | 492 | 68.148 | 10.561 | 4.693 | 1.00 | 43.19 |
| ATOM | 3754 | CA | VAL | 492 | 68.676 | 9.304 | 5.193 | 1.00 | 41.54 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3755 | CB | VAL | 492 | 67.655 | 8.584 | 6.087 | 1.00 | 41.74 |
| ATOM | 3756 | CG1 | VAL | 492 | 68.217 | 7.248 | 6.561 | 1.00 | 43.70 |
| ATOM | 3757 | CG2 | VAL | 492 | 67.283 | 9.463 | 7.269 | 1.00 | 44.07 |
| ATOM | 3758 | C | VAL | 492 | 68.971 | 8.424 | 3.993 | 1.00 | 39.72 |
| ATOM | 3759 | O | VAL | 492 | 68.125 | 8.271 | 3.108 | 1.00 | 39.81 |
| ATOM | 3760 | N | VAL | 493 | 70.176 | 7.872 | 3.942 | 1.00 | 36.38 |
| ATOM | 3762 | CA | VAL | 493 | 70.545 | 7.001 | 2.844 | 1.00 | 35.88 |
| ATOM | 3763 | CB | VAL | 493 | 71.580 | 7.666 | 1.869 | 1.00 | 36.92 |
| ATOM | 3764 | CG1 | VAL | 493 | 71.142 | 9.069 | 1.485 | 1.00 | 36.64 |
| ATOM | 3765 | CG2 | VAL | 493 | 72.978 | 7.670 | 2.469 | 1.00 | 38.29 |
| ATOM | 3766 | C | VAL | 493 | 71.131 | 5.689 | 3.351 | 1.00 | 36.03 |
| ATOM | 3767 | O | VAL | 493 | 71.693 | 5.617 | 4.443 | 1.00 | 36.57 |
| ATOM | 3768 | N | LEU | 494 | 70.947 | 4.637 | 2.571 | 1.00 | 34.91 |
| ATOM | 3770 | CA | LEU | 494 | 71.500 | 3.344 | 2.909 | 1.00 | 36.04 |
| ATOM | 3771 | CB | LEU | 494 | 70.809 | 2.244 | 2.094 | 1.00 | 37.43 |
| ATOM | 3772 | CG | LEU | 494 | 71.312 | 0.814 | 2.269 | 1.00 | 36.62 |
| ATOM | 3773 | CD1 | LEU | 494 | 71.327 | 0.437 | 3.735 | 1.00 | 36.37 |
| ATOM | 3774 | CD2 | LEU | 494 | 70.419 | -0.118 | 1.479 | 1.00 | 40.70 |
| ATOM | 3775 | C | LEU | 494 | 72.967 | 3.451 | 2.510 | 1.00 | 37.08 |
| ATOM | 3776 | O | LEU | 494 | 73.308 | 4.160 | 1.560 | 1.00 | 34.90 |
| ATOM | 3777 | N | ALA | 495 | 73.839 | 2.779 | 3.243 | 1.00 | 37.18 |
| ATOM | 3779 | CA | ALA | 495 | 75.246 | 2.830 | 2.918 | 1.00 | 39.84 |
| ATOM | 3780 | CB | ALA | 495 | 75.885 | 4.066 | 3.541 | 1.00 | 39.29 |
| ATOM | 3781 | C | ALA | 495 | 75.949 | 1.578 | 3.400 | 1.00 | 41.68 |
| ATOM | 3782 | O | ALA | 495 | 75.400 | 0.808 | 4.189 | 1.00 | 41.53 |
| ATOM | 3783 | N | GLU | 496 | 77.149 | 1.348 | 2.881 | 1.00 | 43.44 |
| ATOM | 3785 | CA | GLU | 496 | 77.936 | 0.202 | 3.297 | 1.00 | 42.86 |
| ATOM | 3786 | CB | GLU | 496 | 78.328 | -0.663 | 2.101 | 1.00 | 44.63 |
| ATOM | 3787 | CG | GLU | 496 | 77.120 | -1.167 | 1.320 | 1.00 | 53.31 |
| ATOM | 3788 | CD | GLU | 496 | 77.386 | -2.450 | 0.545 | 1.00 | 59.48 |
| ATOM | 3789 | OE1 | GLU | 496 | 76.494 | -3.332 | 0.534 | 1.00 | 62.39 |
| ATOM | 3790 | OE2 | GLU | 496 | 78.477 | -2.580 | -0.053 | 1.00 | 62.15 |
| ATOM | 3791 | C | GLU | 496 | 79.150 | 0.750 | 4.006 | 1.00 | 40.96 |
| ATOM | 3792 | O | GLU | 496 | 79.889 | 1.568 | 3.455 | 1.00 | 40.81 |
| ATOM | 3793 | N | ALA | 497 | 79.267 | 0.411 | 5.280 | 1.00 | 40.79 |
| ATOM | 3795 | CA | ALA | 497 | 80.381 | 0.857 | 6.096 | 1.00 | 41.84 |
| ATOM | 3796 | CB | ALA | 497 | 79.888 | 1.240 | 7.478 | 1.00 | 38.80 |
| ATOM | 3797 | C | ALA | 497 | 81.394 | -0.280 | 6.181 | 1.00 | 44.72 |
| ATOM | 3798 | O | ALA | 497 | 81.019 | -1.445 | 6.215 | 1.00 | 44.78 |
| ATOM | 3799 | N | ILE | 498 | 82.678 | 0.054 | 6.183 | 1.00 | 48.03 |
| ATOM | 3801 | CA | ILE | 498 | 83.729 | -0.952 | 6.255 | 1.00 | 48.78 |
| ATOM | 3802 | CB | ILE | 498 | 84.654 | -0.894 | 5.014 | 1.00 | 50.57 |
| ATOM | 3803 | CG2 | ILE | 498 | 85.748 | -1.954 | 5.119 | 1.00 | 51.32 |
| ATOM | 3804 | CG1 | ILE | 498 | 83.851 | -1.103 | 3.726 | 1.00 | 51.90 |
| ATOM | 3805 | CD1 | ILE | 498 | 83.139 | 0.146 | 3.198 | 1.00 | 55.47 |
| ATOM | 3806 | C | ILE | 498 | 84.573 | -0.754 | 7.511 | 1.00 | 48.31 |
| ATOM | 3807 | O | ILE | 498 | 85.005 | 0.359 | 7.805 | 1.00 | 47.90 |
| ATOM | 3808 | N | GLY | 499 | 84.754 | -1.829 | 8.271 | 1.00 | 49.29 |
| ATOM | 3810 | CA | GLY | 499 | 85.563 | -1.774 | 9.479 | 1.00 | 53.17 |
| ATOM | 3811 | C | GLY | 499 | 85.076 | -0.944 | 10.657 | 1.00 | 57.22 |
| ATOM | 3812 | O | GLY | 499 | 85.885 | -0.341 | 11.364 | 1.00 | 59.20 |
| ATOM | 3813 | N | LEU | 500 | 83.768 | -0.948 | 10.909 | 1.00 | 58.51 |
| ATOM | 3815 | CA | LEU | 500 | 83.193 | -0.189 | 12.025 | 1.00 | 57.80 |
| ATOM | 3816 | CB | LEU | 500 | 81.705 | -0.519 | 12.181 | 1.00 | 55.67 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3817 | CG | LEU | 500 | 80.789 | 0.036 | 11.086 | 1.00 | 54.81 |
| ATOM | 3818 | CD1 | LEU | 500 | 79.361 | -0.445 | 11.293 | 1.00 | 53.00 |
| ATOM | 3819 | CD2 | LEU | 500 | 80.854 | 1.561 | 11.089 | 1.00 | 53.27 |
| ATOM | 3820 | C | LEU | 500 | 83.926 | -0.466 | 13.333 | 1.00 | 58.15 |
| ATOM | 3821 | O | LEU | 500 | 84.461 | -1.560 | 13.529 | 1.00 | 60.29 |
| ATOM | 3822 | N | PRO | 505 | 87.397 | -6.022 | 10.511 | 1.00 | 77.18 |
| ATOM | 3823 | CD | PRO | 505 | 88.509 | -6.651 | 11.242 | 1.00 | 78.26 |
| ATOM | 3824 | CA | PRO | 505 | 87.755 | -4.660 | 10.097 | 1.00 | 75.62 |
| ATOM | 3825 | CB | PRO | 505 | 89.166 | -4.487 | 10.669 | 1.00 | 75.77 |
| ATOM | 3826 | CG | PRO | 505 | 89.696 | -5.884 | 10.715 | 1.00 | 77.07 |
| ATOM | 3827 | C | PRO | 505 | 87.709 | -4.440 | 8.583 | 1.00 | 73.15 |
| ATOM | 3828 | O | PRO | 505 | 87.772 | -3.308 | 8.105 | 1.00 | 72.63 |
| ATOM | 3829 | N | ASN | 506 | 87.595 | -5.524 | 7.830 | 1.00 | 71.27 |
| ATOM | 3831 | CA | ASN | 506 | 87.518 | -5.421 | 6.380 | 1.00 | 69.14 |
| ATOM | 3832 | CB | ASN | 506 | 88.577 | -6.313 | 5.728 | 1.00 | 70.76 |
| ATOM | 3833 | C | ASN | 506 | 86.119 | -5.840 | 5.940 | 1.00 | 67.30 |
| ATOM | 3834 | O | ASN | 506 | 85.834 | -5.957 | 4.750 | 1.00 | 67.03 |
| ATOM | 3835 | N | ARG | 507 | 85.250 | -6.064 | 6.921 | 1.00 | 65.27 |
| ATOM | 3837 | CA | ARG | 507 | 83.876 | -6.479 | 6.669 | 1.00 | 62.86 |
| ATOM | 3838 | CB | ARG | 507 | 83.335 | -7.267 | 7.864 | 1.00 | 65.45 |
| ATOM | 3839 | C | ARG | 507 | 82.991 | -5.274 | 6.443 | 1.00 | 59.56 |
| ATOM | 3840 | O | ARG | 507 | 83.161 | -4.247 | 7.100 | 1.00 | 59.70 |
| ATOM | 3841 | N | VAL | 508 | 82.057 | -5.397 | 5.509 | 1.00 | 56.65 |
| ATOM | 3843 | CA | VAL | 508 | 81.135 | -4.310 | 5.226 | 1.00 | 55.48 |
| ATOM | 3844 | CB | VAL | 508 | 80.850 | -4.157 | 3.719 | 1.00 | 55.71 |
| ATOM | 3845 | CG1 | VAL | 508 | 82.146 | -3.962 | 2.962 | 1.00 | 58.18 |
| ATOM | 3846 | CG2 | VAL | 508 | 80.096 | -5.356 | 3.188 | 1.00 | 58.76 |
| ATOM | 3847 | C | VAL | 508 | 79.833 | -4.537 | 5.979 | 1.00 | 53.10 |
| ATOM | 3848 | O | VAL | 508 | 79.352 | -5.665 | 6.091 | 1.00 | 54.25 |
| ATOM | 3849 | N | THR | 509 | 79.282 | -3.460 | 6.514 | 1.00 | 50.06 |
| ATOM | 3851 | CA | THR | 509 | 78.041 | -3.512 | 7.260 | 1.00 | 45.70 |
| ATOM | 3852 | CB | THR | 509 | 78.256 | -3.029 | 8.715 | 1.00 | 45.59 |
| ATOM | 3853 | OG1 | THR | 509 | 79.395 | -3.696 | 9.279 | 1.00 | 43.86 |
| ATOM | 3855 | CG2 | THR | 509 | 77.028 | -3.328 | 9.573 | 1.00 | 44.19 |
| ATOM | 3856 | C | THR | 509 | 77.064 | -2.574 | 6.564 | 1.00 | 43.57 |
| ATOM | 3857 | O | THR | 509 | 77.416 | -1.444 | 6.221 | 1.00 | 41.15 |
| ATOM | 3858 | N | LYS | 510 | 75.871 | -3.073 | 6.268 | 1.00 | 42.96 |
| ATOM | 3860 | CA | LYS | 510 | 74.847 | -2.253 | 5.640 | 1.00 | 41.91 |
| ATOM | 3861 | CB | LYS | 510 | 73.740 | -3.144 | 5.091 | 1.00 | 44.74 |
| ATOM | 3862 | CG | LYS | 510 | 72.864 | -2.461 | 4.069 | 1.00 | 51.83 |
| ATOM | 3863 | CD | LYS | 510 | 73.392 | -2.645 | 2.659 | 1.00 | 55.00 |
| ATOM | 3864 | CE | LYS | 510 | 72.769 | -3.879 | 2.020 | 1.00 | 58.36 |
| ATOM | 3865 | NZ | LYS | 510 | 73.069 | -5.131 | 2.769 | 1.00 | 58.57 |
| ATOM | 3869 | C | LYS | 510 | 74.322 | -1.367 | 6.789 | 1.00 | 40.74 |
| ATOM | 3870 | O | LYS | 510 | 73.909 | -1.874 | 7.837 | 1.00 | 40.26 |
| ATOM | 3871 | N | VAL | 511 | 74.413 | -0.052 | 6.624 | 1.00 | 37.21 |
| ATOM | 3873 | CA | VAL | 511 | 73.989 | 0.877 | 7.661 | 1.00 | 33.44 |
| ATOM | 3874 | CB | VAL | 511 | 75.227 | 1.515 | 8.362 | 1.00 | 34.53 |
| ATOM | 3875 | CG1 | VAL | 511 | 76.100 | 0.436 | 9.014 | 1.00 | 31.98 |
| ATOM | 3876 | CG2 | VAL | 511 | 76.048 | 2.322 | 7.358 | 1.00 | 34.82 |
| ATOM | 3877 | C | VAL | 511 | 73.134 | 1.989 | 7.087 | 1.00 | 31.34 |
| ATOM | 3878 | O | VAL | 511 | 73.025 | 2.130 | 5.871 | 1.00 | 31.33 |
| ATOM | 3879 | N | ALA | 512 | 72.485 | 2.748 | 7.961 | 1.00 | 30.70 |
| ATOM | 3881 | CA | ALA | 512 | 71.671 | 3.876 | 7.523 | 1.00 | 30.81 |

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ATOM   3882  CB   ALA  512    70.305   3.879   8.206  1.00  29.85
ATOM   3883  C    ALA  512    72.453   5.124   7.904  1.00  31.30
ATOM   3884  O    ALA  512    73.036   5.197   8.996  1.00  30.24
ATOM   3885  N    VAL  513    72.480   6.096   6.999  1.00  30.86
ATOM   3887  CA   VAL  513    73.208   7.332   7.238  1.00  30.58
ATOM   3888  CB   VAL  513    74.358   7.525   6.223  1.00  31.11
ATOM   3889  CG1  VAL  513    75.132   8.788   6.547  1.00  29.63
ATOM   3890  CG2  VAL  513    75.290   6.317   6.223  1.00  28.70
ATOM   3891  C    VAL  513    72.300   8.556   7.189  1.00  31.28
ATOM   3892  O    VAL  513    71.645   8.824   6.167  1.00  30.12
ATOM   3893  N    LYS  514    72.229   9.257   8.321  1.00  31.03
ATOM   3895  CA   LYS  514    71.439  10.479   8.451  1.00  32.56
ATOM   3896  CB   LYS  514    70.881  10.635   9.870  1.00  34.31
ATOM   3897  CG   LYS  514    69.977   9.516  10.326  1.00  38.25
ATOM   3898  CD   LYS  514    69.513   9.774  11.753  1.00  47.74
ATOM   3899  CE   LYS  514    68.514   8.719  12.230  1.00  51.60
ATOM   3900  NZ   LYS  514    67.226   8.755  11.468  1.00  58.53
ATOM   3904  C    LYS  514    72.357  11.659   8.137  1.00  30.29
ATOM   3905  O    LYS  514    73.485  11.736   8.628  1.00  28.14
ATOM   3906  N    MET  515    71.867  12.580   7.320  1.00  30.67
ATOM   3908  CA   MET  515    72.643  13.747   6.920  1.00  29.94
ATOM   3909  CB   MET  515    73.435  13.442   5.648  1.00  30.64
ATOM   3910  CG   MET  515    72.557  13.038   4.464  1.00  32.16
ATOM   3911  SD   MET  515    73.525  12.522   3.036  1.00  37.59
ATOM   3912  CE   MET  515    74.015  10.933   3.563  1.00  29.11
ATOM   3913  C    MET  515    71.675  14.869   6.635  1.00  29.71
ATOM   3914  O    MET  515    70.462  14.664   6.598  1.00  30.04
ATOM   3915  N    LEU  516    72.212  16.060   6.445  1.00  29.56
ATOM   3917  CA   LEU  516    71.381  17.206   6.136  1.00  30.76
ATOM   3918  CB   LEU  516    72.093  18.508   6.526  1.00  28.20
ATOM   3919  CG   LEU  516    72.396  18.724   8.011  1.00  28.48
ATOM   3920  CD1  LEU  516    73.202  19.983   8.185  1.00  27.55
ATOM   3921  CD2  LEU  516    71.114  18.814   8.794  1.00  25.49
ATOM   3922  C    LEU  516    71.081  17.225   4.647  1.00  30.97
ATOM   3923  O    LEU  516    71.728  16.534   3.851  1.00  29.93
ATOM   3924  N    LYS  517    70.030  17.946   4.291  1.00  31.57
ATOM   3926  CA   LYS  517    69.677  18.117   2.899  1.00  31.44
ATOM   3927  CB   LYS  517    68.169  18.310   2.752  1.00  34.79
ATOM   3928  CG   LYS  517    67.375  17.098   3.194  1.00  38.42
ATOM   3929  CD   LYS  517    66.148  16.888   2.343  1.00  46.52
ATOM   3930  CE   LYS  517    65.087  17.950   2.582  1.00  53.77
ATOM   3931  NZ   LYS  517    63.901  17.740   1.690  1.00  56.38
ATOM   3935  C    LYS  517    70.457  19.377   2.499  1.00  30.18
ATOM   3936  O    LYS  517    70.892  20.134   3.370  1.00  27.47
ATOM   3937  N    SER  518    70.646  19.594   1.201  1.00  31.13
ATOM   3939  CA   SER  518    71.394  20.747   0.693  1.00  32.11
ATOM   3940  CB   SER  518    71.518  20.652  -0.824  1.00  33.45
ATOM   3941  OG   SER  518    70.242  20.567  -1.428  1.00  34.51
ATOM   3943  C    SER  518    70.814  22.103   1.073  1.00  32.81
ATOM   3944  O    SER  518    71.515  23.123   1.027  1.00  34.03
ATOM   3945  N    ASP  519    69.540  22.117   1.449  1.00  29.80
ATOM   3947  CA   ASP  519    68.886  23.354   1.836  1.00  28.94
ATOM   3948  CB   ASP  519    67.473  23.421   1.237  1.00  33.90
ATOM   3949  CG   ASP  519    66.542  22.332   1.771  1.00  34.42
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3950 | OD1 | ASP | 519 | 67.020 | 21.328 | 2.333 | 1.00 | 35.58 |
| ATOM | 3951 | OD2 | ASP | 519 | 65.313 | 22.485 | 1.617 | 1.00 | 41.83 |
| ATOM | 3952 | C | ASP | 519 | 68.829 | 23.559 | 3.342 | 1.00 | 29.08 |
| ATOM | 3953 | O | ASP | 519 | 68.177 | 24.485 | 3.816 | 1.00 | 29.79 |
| ATOM | 3954 | N | ALA | 520 | 69.514 | 22.710 | 4.099 | 1.00 | 29.73 |
| ATOM | 3956 | CA | ALA | 520 | 69.488 | 22.824 | 5.558 | 1.00 | 29.16 |
| ATOM | 3957 | CB | ALA | 520 | 70.174 | 21.639 | 6.190 | 1.00 | 28.13 |
| ATOM | 3958 | C | ALA | 520 | 70.122 | 24.108 | 6.040 | 1.00 | 28.06 |
| ATOM | 3959 | O | ALA | 520 | 70.880 | 24.741 | 5.309 | 1.00 | 28.84 |
| ATOM | 3960 | N | THR | 521 | 69.800 | 24.491 | 7.272 | 1.00 | 27.84 |
| ATOM | 3962 | CA | THR | 521 | 70.357 | 25.692 | 7.885 | 1.00 | 30.45 |
| ATOM | 3963 | CB | THR | 521 | 69.254 | 26.635 | 8.463 | 1.00 | 33.56 |
| ATOM | 3964 | OG1 | THR | 521 | 68.547 | 25.968 | 9.520 | 1.00 | 36.27 |
| ATOM | 3966 | CG2 | THR | 521 | 68.275 | 27.074 | 7.379 | 1.00 | 36.06 |
| ATOM | 3967 | C | THR | 521 | 71.251 | 25.263 | 9.048 | 1.00 | 30.04 |
| ATOM | 3968 | O | THR | 521 | 71.348 | 24.072 | 9.369 | 1.00 | 28.16 |
| ATOM | 3969 | N | GLU | 522 | 71.876 | 26.241 | 9.696 | 1.00 | 31.42 |
| ATOM | 3971 | CA | GLU | 522 | 72.745 | 25.978 | 10.832 | 1.00 | 36.94 |
| ATOM | 3972 | CB | GLU | 522 | 73.404 | 27.282 | 11.299 | 1.00 | 44.74 |
| ATOM | 3973 | CG | GLU | 522 | 74.414 | 27.130 | 12.450 | 1.00 | 58.34 |
| ATOM | 3974 | CD | GLU | 522 | 75.769 | 26.579 | 12.009 | 1.00 | 64.50 |
| ATOM | 3975 | OE1 | GLU | 522 | 76.798 | 27.261 | 12.231 | 1.00 | 64.89 |
| ATOM | 3976 | OE2 | GLU | 522 | 75.806 | 25.461 | 11.452 | 1.00 | 70.26 |
| ATOM | 3977 | C | GLU | 522 | 71.932 | 25.345 | 11.969 | 1.00 | 34.02 |
| ATOM | 3978 | O | GLU | 522 | 72.428 | 24.480 | 12.684 | 1.00 | 31.11 |
| ATOM | 3979 | N | LYS | 523 | 70.670 | 25.750 | 12.097 | 1.00 | 32.53 |
| ATOM | 3981 | CA | LYS | 523 | 69.805 | 25.210 | 13.135 | 1.00 | 34.06 |
| ATOM | 3982 | CB | LYS | 523 | 68.481 | 25.970 | 13.188 | 1.00 | 39.54 |
| ATOM | 3983 | CG | LYS | 523 | 67.560 | 25.541 | 14.322 | 1.00 | 45.55 |
| ATOM | 3984 | CD | LYS | 523 | 66.360 | 24.776 | 13.789 | 1.00 | 52.08 |
| ATOM | 3985 | CE | LYS | 523 | 65.443 | 24.312 | 14.914 | 1.00 | 54.16 |
| ATOM | 3986 | NZ | LYS | 523 | 64.313 | 23.509 | 14.373 | 1.00 | 54.38 |
| ATOM | 3990 | C | LYS | 523 | 69.572 | 23.733 | 12.861 | 1.00 | 31.73 |
| ATOM | 3991 | O | LYS | 523 | 69.589 | 22.922 | 13.788 | 1.00 | 31.15 |
| ATOM | 3992 | N | ASP | 524 | 69.374 | 23.383 | 11.590 | 1.00 | 29.22 |
| ATOM | 3994 | CA | ASP | 524 | 69.182 | 21.980 | 11.214 | 1.00 | 28.79 |
| ATOM | 3995 | CB | ASP | 524 | 68.928 | 21.831 | 9.714 | 1.00 | 27.65 |
| ATOM | 3996 | CG | ASP | 524 | 67.586 | 22.396 | 9.286 | 1.00 | 33.89 |
| ATOM | 3997 | OD1 | ASP | 524 | 66.568 | 22.106 | 9.954 | 1.00 | 34.66 |
| ATOM | 3998 | OD2 | ASP | 524 | 67.549 | 23.120 | 8.270 | 1.00 | 30.04 |
| ATOM | 3999 | C | ASP | 524 | 70.424 | 21.190 | 11.606 | 1.00 | 28.00 |
| ATOM | 4000 | O | ASP | 524 | 70.317 | 20.104 | 12.162 | 1.00 | 30.83 |
| ATOM | 4001 | N | LEU | 525 | 71.603 | 21.761 | 11.347 | 1.00 | 29.87 |
| ATOM | 4003 | CA | LEU | 525 | 72.873 | 21.121 | 11.700 | 1.00 | 27.60 |
| ATOM | 4004 | CB | LEU | 525 | 74.064 | 21.997 | 11.282 | 1.00 | 24.08 |
| ATOM | 4005 | CG | LEU | 525 | 75.462 | 21.433 | 11.593 | 1.00 | 26.11 |
| ATOM | 4006 | CD1 | LEU | 525 | 75.597 | 19.979 | 11.098 | 1.00 | 23.67 |
| ATOM | 4007 | CD2 | LEU | 525 | 76.530 | 22.321 | 10.967 | 1.00 | 21.28 |
| ATOM | 4008 | C | LEU | 525 | 72.909 | 20.869 | 13.200 | 1.00 | 26.38 |
| ATOM | 4009 | O | LEU | 525 | 73.249 | 19.777 | 13.653 | 1.00 | 26.09 |
| ATOM | 4010 | N | SER | 526 | 72.560 | 21.902 | 13.956 | 1.00 | 29.72 |
| ATOM | 4012 | CA | SER | 526 | 72.500 | 21.861 | 15.422 | 1.00 | 32.16 |
| ATOM | 4013 | CB | SER | 526 | 71.980 | 23.209 | 15.939 | 1.00 | 33.45 |
| ATOM | 4014 | OG | SER | 526 | 71.793 | 23.213 | 17.343 | 1.00 | 40.42 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4016 | C | SER | 526 | 71.572 | 20.728 | 15.902 | 1.00 | 31.64 |
| ATOM | 4017 | O | SER | 526 | 71.869 | 20.030 | 16.889 | 1.00 | 32.54 |
| ATOM | 4018 | N | ASP | 527 | 70.454 | 20.561 | 15.201 | 1.00 | 27.92 |
| ATOM | 4020 | CA | ASP | 527 | 69.492 | 19.527 | 15.524 | 1.00 | 28.60 |
| ATOM | 4021 | CB | ASP | 527 | 68.187 | 19.767 | 14.765 | 1.00 | 29.35 |
| ATOM | 4022 | CG | ASP | 527 | 67.418 | 20.984 | 15.278 | 1.00 | 31.37 |
| ATOM | 4023 | OD1 | ASP | 527 | 67.759 | 21.549 | 16.353 | 1.00 | 31.96 |
| ATOM | 4024 | OD2 | ASP | 527 | 66.456 | 21.369 | 14.591 | 1.00 | 32.58 |
| ATOM | 4025 | C | ASP | 527 | 70.038 | 18.131 | 15.246 | 1.00 | 28.82 |
| ATOM | 4026 | O | ASP | 527 | 69.854 | 17.212 | 16.047 | 1.00 | 29.65 |
| ATOM | 4027 | N | LEU | 528 | 70.721 | 17.962 | 14.120 | 1.00 | 29.29 |
| ATOM | 4029 | CA | LEU | 528 | 71.302 | 16.658 | 13.794 | 1.00 | 29.94 |
| ATOM | 4030 | CB | LEU | 528 | 71.780 | 16.621 | 12.336 | 1.00 | 26.45 |
| ATOM | 4031 | CG | LEU | 528 | 72.315 | 15.276 | 11.840 | 1.00 | 28.34 |
| ATOM | 4032 | CD1 | LEU | 528 | 71.240 | 14.189 | 12.035 | 1.00 | 27.16 |
| ATOM | 4033 | CD2 | LEU | 528 | 72.756 | 15.387 | 10.372 | 1.00 | 25.91 |
| ATOM | 4034 | C | LEU | 528 | 72.449 | 16.319 | 14.776 | 1.00 | 29.72 |
| ATOM | 4035 | O | LEU | 528 | 72.617 | 15.162 | 15.178 | 1.00 | 28.98 |
| ATOM | 4036 | N | ILE | 529 | 73.224 | 17.329 | 15.168 | 1.00 | 30.15 |
| ATOM | 4038 | CA | ILE | 529 | 74.305 | 17.131 | 16.134 | 1.00 | 28.88 |
| ATOM | 4039 | CB | ILE | 529 | 75.188 | 18.382 | 16.268 | 1.00 | 26.91 |
| ATOM | 4040 | CG2 | ILE | 529 | 76.175 | 18.221 | 17.423 | 1.00 | 24.82 |
| ATOM | 4041 | CG1 | ILE | 529 | 75.960 | 18.613 | 14.984 | 1.00 | 23.98 |
| ATOM | 4042 | CD1 | ILE | 529 | 76.663 | 19.932 | 14.973 | 1.00 | 28.33 |
| ATOM | 4043 | C | ILE | 529 | 73.709 | 16.799 | 17.518 | 1.00 | 29.71 |
| ATOM | 4044 | O | ILE | 529 | 74.172 | 15.880 | 18.193 | 1.00 | 29.19 |
| ATOM | 4045 | N | SER | 530 | 72.672 | 17.524 | 17.926 | 1.00 | 26.84 |
| ATOM | 4047 | CA | SER | 530 | 72.061 | 17.247 | 19.214 | 1.00 | 31.46 |
| ATOM | 4048 | CB | SER | 530 | 70.948 | 18.251 | 19.521 | 1.00 | 36.17 |
| ATOM | 4049 | OG | SER | 530 | 70.045 | 18.363 | 18.431 | 1.00 | 47.58 |
| ATOM | 4051 | C | SER | 530 | 71.526 | 15.822 | 19.248 | 1.00 | 30.05 |
| ATOM | 4052 | O | SER | 530 | 71.646 | 15.136 | 20.270 | 1.00 | 29.61 |
| ATOM | 4053 | N | GLU | 531 | 70.972 | 15.357 | 18.132 | 1.00 | 27.74 |
| ATOM | 4055 | CA | GLU | 531 | 70.458 | 13.999 | 18.090 | 1.00 | 28.71 |
| ATOM | 4056 | CB | GLU | 531 | 69.709 | 13.727 | 16.789 | 1.00 | 29.72 |
| ATOM | 4057 | CG | GLU | 531 | 69.147 | 12.319 | 16.737 | 1.00 | 32.21 |
| ATOM | 4058 | CD | GLU | 531 | 68.510 | 11.979 | 15.414 | 1.00 | 33.88 |
| ATOM | 4059 | OE1 | GLU | 531 | 68.026 | 10.846 | 15.281 | 1.00 | 37.60 |
| ATOM | 4060 | OE2 | GLU | 531 | 68.483 | 12.833 | 14.510 | 1.00 | 34.70 |
| ATOM | 4061 | C | GLU | 531 | 71.578 | 12.974 | 18.271 | 1.00 | 28.91 |
| ATOM | 4062 | O | GLU | 531 | 71.428 | 12.007 | 19.019 | 1.00 | 29.46 |
| ATOM | 4063 | N | MET | 532 | 72.686 | 13.179 | 17.567 | 1.00 | 28.84 |
| ATOM | 4065 | CA | MET | 532 | 73.851 | 12.296 | 17.648 | 1.00 | 29.35 |
| ATOM | 4066 | CB | MET | 532 | 74.948 | 12.786 | 16.689 | 1.00 | 27.41 |
| ATOM | 4067 | CG | MET | 532 | 76.299 | 12.117 | 16.872 | 1.00 | 26.71 |
| ATOM | 4068 | SD | MET | 532 | 77.503 | 12.675 | 15.640 | 1.00 | 32.27 |
| ATOM | 4069 | CE | MET | 532 | 77.732 | 14.400 | 16.117 | 1.00 | 24.10 |
| ATOM | 4070 | C | MET | 532 | 74.389 | 12.280 | 19.078 | 1.00 | 28.80 |
| ATOM | 4071 | O | MET | 532 | 74.700 | 11.230 | 19.630 | 1.00 | 29.74 |
| ATOM | 4072 | N | GLU | 533 | 74.481 | 13.454 | 19.681 | 1.00 | 28.83 |
| ATOM | 4074 | CA | GLU | 533 | 74.985 | 13.546 | 21.033 | 1.00 | 29.66 |
| ATOM | 4075 | CB | GLU | 533 | 75.182 | 15.008 | 21.423 | 1.00 | 32.23 |
| ATOM | 4076 | CG | GLU | 533 | 76.331 | 15.687 | 20.651 | 1.00 | 34.47 |
| ATOM | 4077 | CD | GLU | 533 | 77.656 | 14.937 | 20.774 | 1.00 | 38.03 |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4078 | OE1 | GLU | 533 | 78.168 | 14.780 | 21.903 | 1.00 | 39.75 | |
| ATOM | 4079 | OE2 | GLU | 533 | 78.192 | 14.497 | 19.736 | 1.00 | 38.75 | |
| ATOM | 4080 | C | GLU | 533 | 74.058 | 12.815 | 22.005 | 1.00 | 31.55 | |
| ATOM | 4081 | O | GLU | 533 | 74.521 | 12.083 | 22.889 | 1.00 | 30.63 | |
| ATOM | 4082 | N | MET | 534 | 72.750 | 12.958 | 21.799 | 1.00 | 31.31 | |
| ATOM | 4084 | CA | MET | 534 | 71.789 | 12.289 | 22.664 | 1.00 | 30.78 | |
| ATOM | 4085 | CB | MET | 534 | 70.348 | 12.672 | 22.319 | 1.00 | 31.23 | |
| ATOM | 4086 | CG | MET | 534 | 69.453 | 12.648 | 23.551 | 0.50 | 29.35 | PRT1 |
| ATOM | 4087 | SD | MET | 534 | 67.688 | 12.563 | 23.246 | 0.50 | 28.79 | PRT1 |
| ATOM | 4088 | CE | MET | 534 | 67.290 | 14.230 | 22.875 | 0.50 | 26.96 | PRT1 |
| ATOM | 4089 | C | MET | 534 | 71.991 | 10.773 | 22.560 | 1.00 | 28.82 | |
| ATOM | 4090 | O | MET | 534 | 72.053 | 10.083 | 23.568 | 1.00 | 30.10 | |
| ATOM | 4091 | N | MET | 535 | 72.149 | 10.271 | 21.339 | 1.00 | 29.16 | |
| ATOM | 4093 | CA | MET | 535 | 72.381 | 8.852 | 21.110 | 1.00 | 29.37 | |
| ATOM | 4094 | CB | MET | 535 | 72.546 | 8.551 | 19.617 | 1.00 | 27.35 | |
| ATOM | 4095 | CG | MET | 535 | 71.281 | 8.790 | 18.817 | 1.00 | 28.40 | |
| ATOM | 4096 | SD | MET | 535 | 71.255 | 7.955 | 17.255 | 1.00 | 30.26 | |
| ATOM | 4097 | CE | MET | 535 | 71.336 | 9.279 | 16.188 | 1.00 | 35.50 | |
| ATOM | 4098 | C | MET | 535 | 73.612 | 8.388 | 21.887 | 1.00 | 30.36 | |
| ATOM | 4099 | O | MET | 535 | 73.626 | 7.287 | 22.460 | 1.00 | 26.13 | |
| ATOM | 4100 | N | LYS | 536 | 74.640 | 9.233 | 21.909 | 1.00 | 30.70 | |
| ATOM | 4102 | CA | LYS | 536 | 75.850 | 8.913 | 22.649 | 1.00 | 31.76 | |
| ATOM | 4103 | CB | LYS | 536 | 76.934 | 9.954 | 22.388 | 1.00 | 31.05 | |
| ATOM | 4104 | CG | LYS | 536 | 77.550 | 9.883 | 21.004 | 1.00 | 26.80 | |
| ATOM | 4105 | CD | LYS | 536 | 78.534 | 11.017 | 20.860 | 1.00 | 31.05 | |
| ATOM | 4106 | CE | LYS | 536 | 79.132 | 11.138 | 19.466 | 1.00 | 29.83 | |
| ATOM | 4107 | NZ | LYS | 536 | 79.957 | 12.377 | 19.440 | 1.00 | 29.32 | |
| ATOM | 4111 | C | LYS | 536 | 75.550 | 8.834 | 24.150 | 1.00 | 31.99 | |
| ATOM | 4112 | O | LYS | 536 | 75.920 | 7.859 | 24.806 | 1.00 | 31.92 | |
| ATOM | 4113 | N | MET | 537 | 74.837 | 9.826 | 24.676 | 1.00 | 31.81 | |
| ATOM | 4115 | CA | MET | 537 | 74.517 | 9.835 | 26.090 | 1.00 | 35.37 | |
| ATOM | 4116 | CB | MET | 537 | 73.860 | 11.154 | 26.506 | 1.00 | 41.32 | |
| ATOM | 4117 | CG | MET | 537 | 74.828 | 12.335 | 26.610 | 1.00 | 51.50 | |
| ATOM | 4118 | SD | MET | 537 | 76.234 | 12.090 | 27.776 | 1.00 | 57.48 | |
| ATOM | 4119 | CE | MET | 537 | 75.460 | 12.637 | 29.334 | 1.00 | 56.91 | |
| ATOM | 4120 | C | MET | 537 | 73.630 | 8.679 | 26.499 | 1.00 | 36.11 | |
| ATOM | 4121 | O | MET | 537 | 73.845 | 8.084 | 27.548 | 1.00 | 38.54 | |
| ATOM | 4122 | N | ILE | 538 | 72.652 | 8.347 | 25.661 | 1.00 | 33.69 | |
| ATOM | 4124 | CA | ILE | 538 | 71.704 | 7.277 | 25.954 | 1.00 | 31.62 | |
| ATOM | 4125 | CB | ILE | 538 | 70.492 | 7.314 | 24.974 | 1.00 | 28.21 | |
| ATOM | 4126 | CG2 | ILE | 538 | 69.681 | 6.013 | 25.034 | 1.00 | 28.22 | |
| ATOM | 4127 | CG1 | ILE | 538 | 69.590 | 8.488 | 25.338 | 1.00 | 23.74 | |
| ATOM | 4128 | CD1 | ILE | 538 | 68.487 | 8.728 | 24.344 | 1.00 | 27.94 | |
| ATOM | 4129 | C | ILE | 538 | 72.322 | 5.894 | 26.008 | 1.00 | 31.07 | |
| ATOM | 4130 | O | ILE | 538 | 71.952 | 5.080 | 26.860 | 1.00 | 33.13 | |
| ATOM | 4131 | N | GLY | 539 | 73.239 | 5.611 | 25.094 | 1.00 | 29.52 | |
| ATOM | 4133 | CA | GLY | 539 | 73.871 | 4.309 | 25.093 | 1.00 | 28.40 | |
| ATOM | 4134 | C | GLY | 539 | 73.111 | 3.275 | 24.289 | 1.00 | 30.21 | |
| ATOM | 4135 | O | GLY | 539 | 72.018 | 3.554 | 23.788 | 1.00 | 29.66 | |
| ATOM | 4136 | N | LYS | 540 | 73.679 | 2.074 | 24.199 | 1.00 | 28.44 | |
| ATOM | 4138 | CA | LYS | 540 | 73.105 | 0.984 | 23.426 | 1.00 | 31.09 | |
| ATOM | 4139 | CB | LYS | 540 | 74.215 | 0.089 | 22.895 | 1.00 | 33.15 | |
| ATOM | 4140 | CG | LYS | 540 | 75.116 | 0.776 | 21.906 | 1.00 | 39.54 | |
| ATOM | 4141 | CD | LYS | 540 | 76.125 | -0.175 | 21.329 | 1.00 | 43.98 | |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4142 | CE | LYS | 540 | 77.033 | 0.562 | 20.349 | 1.00 | 50.79 |
| ATOM | 4143 | NZ | LYS | 540 | 76.338 | 0.977 | 19.086 | 1.00 | 51.09 |
| ATOM | 4147 | C | LYS | 540 | 72.053 | 0.087 | 24.059 | 1.00 | 32.78 |
| ATOM | 4148 | O | LYS | 540 | 72.088 | -0.195 | 25.266 | 1.00 | 32.41 |
| ATOM | 4149 | N | HIS | 541 | 71.137 | -0.374 | 23.208 | 1.00 | 31.20 |
| ATOM | 4151 | CA | HIS | 541 | 70.080 | -1.304 | 23.591 | 1.00 | 31.53 |
| ATOM | 4152 | CB | HIS | 541 | 68.911 | -0.630 | 24.298 | 1.00 | 30.69 |
| ATOM | 4153 | CG | HIS | 541 | 67.948 | -1.613 | 24.882 | 1.00 | 31.18 |
| ATOM | 4154 | CD2 | HIS | 541 | 67.938 | -2.255 | 26.072 | 1.00 | 33.02 |
| ATOM | 4155 | ND1 | HIS | 541 | 66.882 | -2.123 | 24.165 | 1.00 | 30.56 |
| ATOM | 4157 | CE1 | HIS | 541 | 66.268 | -3.037 | 24.889 | 1.00 | 32.95 |
| ATOM | 4158 | NE2 | HIS | 541 | 66.886 | -3.140 | 26.053 | 1.00 | 31.79 |
| ATOM | 4160 | C | HIS | 541 | 69.590 | -2.013 | 22.340 | 1.00 | 32.72 |
| ATOM | 4161 | O | HIS | 541 | 69.495 | -1.404 | 21.275 | 1.00 | 30.34 |
| ATOM | 4162 | N | LYS | 542 | 69.282 | -3.305 | 22.475 | 1.00 | 32.32 |
| ATOM | 4164 | CA | LYS | 542 | 68.828 | -4.131 | 21.359 | 1.00 | 30.29 |
| ATOM | 4165 | CB | LYS | 542 | 68.637 | -5.587 | 21.798 | 1.00 | 29.34 |
| ATOM | 4166 | C | LYS | 542 | 67.560 | -3.661 | 20.692 | 1.00 | 29.09 |
| ATOM | 4167 | O | LYS | 542 | 67.369 | -3.903 | 19.507 | 1.00 | 29.12 |
| ATOM | 4168 | N | ASN | 543 | 66.683 | -3.012 | 21.446 | 1.00 | 28.54 |
| ATOM | 4170 | CA | ASN | 543 | 65.425 | -2.559 | 20.869 | 1.00 | 29.10 |
| ATOM | 4171 | CB | ASN | 543 | 64.245 | -3.047 | 21.712 | 1.00 | 29.69 |
| ATOM | 4172 | CG | ASN | 543 | 64.253 | -4.556 | 21.900 | 1.00 | 29.62 |
| ATOM | 4173 | OD1 | ASN | 543 | 64.510 | -5.050 | 23.000 | 1.00 | 31.63 |
| ATOM | 4174 | ND2 | ASN | 543 | 64.020 | -5.291 | 20.828 | 1.00 | 28.66 |
| ATOM | 4177 | C | ASN | 543 | 65.299 | -1.073 | 20.532 | 1.00 | 29.61 |
| ATOM | 4178 | O | ASN | 543 | 64.207 | -0.507 | 20.578 | 1.00 | 28.00 |
| ATOM | 4179 | N | ILE | 544 | 66.432 | -0.442 | 20.222 | 1.00 | 28.39 |
| ATOM | 4181 | CA | ILE | 544 | 66.466 | 0.958 | 19.804 | 1.00 | 25.73 |
| ATOM | 4182 | CB | ILE | 544 | 66.903 | 1.952 | 20.935 | 1.00 | 25.98 |
| ATOM | 4183 | CG2 | ILE | 544 | 66.083 | 1.721 | 22.215 | 1.00 | 22.04 |
| ATOM | 4184 | CG1 | ILE | 544 | 68.412 | 1.860 | 21.209 | 1.00 | 24.30 |
| ATOM | 4185 | CD1 | ILE | 544 | 68.901 | 2.846 | 22.274 | 1.00 | 22.83 |
| ATOM | 4186 | C | ILE | 544 | 67.463 | 1.020 | 18.639 | 1.00 | 26.20 |
| ATOM | 4187 | O | ILE | 544 | 68.276 | 0.106 | 18.467 | 1.00 | 25.46 |
| ATOM | 4188 | N | ILE | 545 | 67.307 | 2.016 | 17.771 | 1.00 | 26.26 |
| ATOM | 4190 | CA | ILE | 545 | 68.223 | 2.209 | 16.641 | 1.00 | 27.62 |
| ATOM | 4191 | CB | ILE | 545 | 67.647 | 3.195 | 15.585 | 1.00 | 28.33 |
| ATOM | 4192 | CG2 | ILE | 545 | 68.726 | 3.595 | 14.562 | 1.00 | 28.00 |
| ATOM | 4193 | CG1 | ILE | 545 | 66.453 | 2.565 | 14.856 | 1.00 | 24.69 |
| ATOM | 4194 | CD1 | ILE | 545 | 66.850 | 1.467 | 13.875 | 1.00 | 26.17 |
| ATOM | 4195 | C | ILE | 545 | 69.492 | 2.794 | 17.267 | 1.00 | 28.23 |
| ATOM | 4196 | O | ILE | 545 | 69.468 | 3.872 | 17.846 | 1.00 | 28.97 |
| ATOM | 4197 | N | ASN | 546 | 70.595 | 2.069 | 17.164 | 1.00 | 29.45 |
| ATOM | 4199 | CA | ASN | 546 | 71.845 | 2.508 | 17.774 | 1.00 | 28.58 |
| ATOM | 4200 | CB | ASN | 546 | 72.580 | 1.309 | 18.384 | 1.00 | 26.34 |
| ATOM | 4201 | CG | ASN | 546 | 71.812 | 0.673 | 19.527 | 1.00 | 25.52 |
| ATOM | 4202 | OD1 | ASN | 546 | 71.634 | 1.277 | 20.580 | 1.00 | 28.82 |
| ATOM | 4203 | ND2 | ASN | 546 | 71.341 | -0.542 | 19.318 | 1.00 | 26.57 |
| ATOM | 4206 | C | ASN | 546 | 72.810 | 3.264 | 16.881 | 1.00 | 28.74 |
| ATOM | 4207 | O | ASN | 546 | 72.858 | 3.041 | 15.675 | 1.00 | 29.26 |
| ATOM | 4208 | N | LEU | 547 | 73.578 | 4.155 | 17.504 | 1.00 | 29.90 |
| ATOM | 4210 | CA | LEU | 547 | 74.618 | 4.936 | 16.834 | 1.00 | 30.27 |
| ATOM | 4211 | CB | LEU | 547 | 75.075 | 6.081 | 17.745 | 1.00 | 25.85 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4212 | CG | LEU | 547 | 76.161 | 7.034 | 17.232 | 1.00 | 27.73 |
| ATOM | 4213 | CD1 | LEU | 547 | 75.670 | 7.851 | 16.033 | 1.00 | 27.38 |
| ATOM | 4214 | CD2 | LEU | 547 | 76.545 | 7.966 | 18.345 | 1.00 | 29.14 |
| ATOM | 4215 | C | LEU | 547 | 75.811 | 4.004 | 16.567 | 1.00 | 32.22 |
| ATOM | 4216 | O | LEU | 547 | 76.256 | 3.291 | 17.471 | 1.00 | 33.38 |
| ATOM | 4217 | N | LEU | 548 | 76.317 | 4.005 | 15.335 | 1.00 | 32.12 |
| ATOM | 4219 | CA | LEU | 548 | 77.452 | 3.159 | 14.960 | 1.00 | 32.94 |
| ATOM | 4220 | CB | LEU | 548 | 77.103 | 2.310 | 13.740 | 1.00 | 29.97 |
| ATOM | 4221 | CG | LEU | 548 | 75.839 | 1.458 | 13.840 | 1.00 | 31.55 |
| ATOM | 4222 | CD1 | LEU | 548 | 75.662 | 0.713 | 12.540 | 1.00 | 27.85 |
| ATOM | 4223 | CD2 | LEU | 548 | 75.917 | 0.500 | 15.025 | 1.00 | 26.34 |
| ATOM | 4224 | C | LEU | 548 | 78.726 | 3.955 | 14.654 | 1.00 | 36.06 |
| ATOM | 4225 | O | LEU | 548 | 79.836 | 3.410 | 14.668 | 1.00 | 36.42 |
| ATOM | 4226 | N | GLY | 549 | 78.562 | 5.219 | 14.298 | 1.00 | 35.78 |
| ATOM | 4228 | CA | GLY | 549 | 79.713 | 6.042 | 13.987 | 1.00 | 36.22 |
| ATOM | 4229 | C | GLY | 549 | 79.267 | 7.376 | 13.433 | 1.00 | 35.30 |
| ATOM | 4230 | O | GLY | 549 | 78.062 | 7.646 | 13.362 | 1.00 | 33.46 |
| ATOM | 4231 | N | ALA | 550 | 80.232 | 8.206 | 13.042 | 1.00 | 34.94 |
| ATOM | 4233 | CA | ALA | 550 | 79.945 | 9.525 | 12.490 | 1.00 | 31.91 |
| ATOM | 4234 | CB | ALA | 550 | 79.588 | 10.495 | 13.613 | 1.00 | 30.54 |
| ATOM | 4235 | C | ALA | 550 | 81.128 | 10.077 | 11.715 | 1.00 | 31.58 |
| ATOM | 4236 | O | ALA | 550 | 82.281 | 9.832 | 12.080 | 1.00 | 31.23 |
| ATOM | 4237 | N | CYS | 551 | 80.818 | 10.812 | 10.643 | 1.00 | 31.13 |
| ATOM | 4239 | CA | CYS | 551 | 81.805 | 11.503 | 9.804 | 1.00 | 28.28 |
| ATOM | 4240 | CB | CYS | 551 | 81.621 | 11.180 | 8.316 | 1.00 | 27.27 |
| ATOM | 4241 | SG | CYS | 551 | 81.771 | 9.449 | 7.839 | 1.00 | 30.33 |
| ATOM | 4242 | C | CYS | 551 | 81.450 | 12.960 | 10.074 | 1.00 | 25.88 |
| ATOM | 4243 | O | CYS | 551 | 80.432 | 13.458 | 9.605 | 1.00 | 27.73 |
| ATOM | 4244 | N | THR | 552 | 82.214 | 13.586 | 10.954 | 1.00 | 25.35 |
| ATOM | 4246 | CA | THR | 552 | 81.988 | 14.967 | 11.353 | 1.00 | 26.79 |
| ATOM | 4247 | CB | THR | 552 | 82.051 | 15.092 | 12.899 | 1.00 | 27.76 |
| ATOM | 4248 | OG1 | THR | 552 | 83.392 | 14.839 | 13.338 | 1.00 | 27.62 |
| ATOM | 4250 | CG2 | THR | 552 | 81.119 | 14.086 | 13.575 | 1.00 | 29.17 |
| ATOM | 4251 | C | THR | 552 | 83.036 | 15.931 | 10.790 | 1.00 | 25.03 |
| ATOM | 4252 | O | THR | 552 | 82.825 | 17.137 | 10.746 | 1.00 | 25.34 |
| ATOM | 4253 | N | GLN | 553 | 84.174 | 15.385 | 10.381 | 1.00 | 27.34 |
| ATOM | 4255 | CA | GLN | 553 | 85.285 | 16.190 | 9.888 | 1.00 | 26.31 |
| ATOM | 4256 | CB | GLN | 553 | 86.601 | 15.639 | 10.468 | 1.00 | 25.05 |
| ATOM | 4257 | CG | GLN | 553 | 86.581 | 15.491 | 11.993 | 1.00 | 24.78 |
| ATOM | 4258 | CD | GLN | 553 | 86.382 | 16.823 | 12.709 | 1.00 | 25.40 |
| ATOM | 4259 | OE1 | GLN | 553 | 87.175 | 17.748 | 12.546 | 1.00 | 33.74 |
| ATOM | 4260 | NE2 | GLN | 553 | 85.338 | 16.920 | 13.516 | 1.00 | 25.61 |
| ATOM | 4263 | C | GLN | 553 | 85.390 | 16.274 | 8.379 | 1.00 | 27.08 |
| ATOM | 4264 | O | GLN | 553 | 85.083 | 15.318 | 7.669 | 1.00 | 28.76 |
| ATOM | 4265 | N | ASP | 554 | 85.804 | 17.438 | 7.899 | 1.00 | 28.63 |
| ATOM | 4267 | CA | ASP | 554 | 86.015 | 17.677 | 6.471 | 1.00 | 29.70 |
| ATOM | 4268 | CB | ASP | 554 | 87.335 | 17.050 | 6.051 | 1.00 | 29.73 |
| ATOM | 4269 | CG | ASP | 554 | 88.480 | 17.587 | 6.857 | 1.00 | 33.38 |
| ATOM | 4270 | OD1 | ASP | 554 | 88.794 | 18.780 | 6.711 | 1.00 | 36.53 |
| ATOM | 4271 | OD2 | ASP | 554 | 89.024 | 16.841 | 7.687 | 1.00 | 36.40 |
| ATOM | 4272 | C | ASP | 554 | 84.908 | 17.258 | 5.522 | 1.00 | 29.64 |
| ATOM | 4273 | O | ASP | 554 | 85.112 | 16.422 | 4.643 | 1.00 | 32.06 |
| ATOM | 4274 | N | GLY | 555 | 83.748 | 17.881 | 5.679 | 1.00 | 28.59 |
| ATOM | 4276 | CA | GLY | 555 | 82.620 | 17.579 | 4.825 | 1.00 | 26.85 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4277 | C | GLY | 555 | 81.333 | 17.434 | 5.607 | 1.00 | 25.30 |
| ATOM | 4278 | O | GLY | 555 | 81.319 | 17.593 | 6.834 | 1.00 | 23.96 |
| ATOM | 4279 | N | PRO | 556 | 80.229 | 17.113 | 4.920 | 1.00 | 24.84 |
| ATOM | 4280 | CD | PRO | 556 | 80.159 | 16.850 | 3.472 | 1.00 | 21.36 |
| ATOM | 4281 | CA | PRO | 556 | 78.920 | 16.942 | 5.550 | 1.00 | 25.26 |
| ATOM | 4282 | CB | PRO | 556 | 78.033 | 16.494 | 4.386 | 1.00 | 23.37 |
| ATOM | 4283 | CG | PRO | 556 | 79.025 | 15.881 | 3.398 | 1.00 | 24.44 |
| ATOM | 4284 | C | PRO | 556 | 78.885 | 15.941 | 6.700 | 1.00 | 26.50 |
| ATOM | 4285 | O | PRO | 556 | 79.515 | 14.875 | 6.654 | 1.00 | 27.38 |
| ATOM | 4286 | N | LEU | 557 | 78.171 | 16.314 | 7.754 | 1.00 | 26.25 |
| ATOM | 4288 | CA | LEU | 557 | 78.032 | 15.452 | 8.917 | 1.00 | 28.25 |
| ATOM | 4289 | CB | LEU | 557 | 77.403 | 16.217 | 10.092 | 1.00 | 27.09 |
| ATOM | 4290 | CG | LEU | 557 | 76.922 | 15.414 | 11.310 | 1.00 | 28.35 |
| ATOM | 4291 | CD1 | LEU | 557 | 78.088 | 14.733 | 12.011 | 1.00 | 25.54 |
| ATOM | 4292 | CD2 | LEU | 557 | 76.204 | 16.340 | 12.271 | 1.00 | 26.91 |
| ATOM | 4293 | C | LEU | 557 | 77.169 | 14.246 | 8.554 | 1.00 | 29.06 |
| ATOM | 4294 | O | LEU | 557 | 76.060 | 14.385 | 8.011 | 1.00 | 29.05 |
| ATOM | 4295 | N | TYR | 558 | 77.717 | 13.065 | 8.807 | 1.00 | 29.43 |
| ATOM | 4297 | CA | TYR | 558 | 77.018 | 11.823 | 8.573 | 1.00 | 28.02 |
| ATOM | 4298 | CB | TYR | 558 | 77.813 | 10.918 | 7.632 | 1.00 | 27.83 |
| ATOM | 4299 | CG | TYR | 558 | 77.969 | 11.414 | 6.203 | 1.00 | 31.70 |
| ATOM | 4300 | CD1 | TYR | 558 | 78.966 | 10.893 | 5.383 | 1.00 | 32.90 |
| ATOM | 4301 | CE1 | TYR | 558 | 79.121 | 11.315 | 4.073 | 1.00 | 32.69 |
| ATOM | 4302 | CD2 | TYR | 558 | 77.122 | 12.386 | 5.666 | 1.00 | 30.23 |
| ATOM | 4303 | CE2 | TYR | 558 | 77.271 | 12.815 | 4.350 | 1.00 | 29.97 |
| ATOM | 4304 | CZ | TYR | 558 | 78.280 | 12.272 | 3.560 | 1.00 | 33.20 |
| ATOM | 4305 | OH | TYR | 558 | 78.452 | 12.681 | 2.253 | 1.00 | 35.32 |
| ATOM | 4307 | C | TYR | 558 | 76.848 | 11.131 | 9.932 | 1.00 | 28.42 |
| ATOM | 4308 | O | TYR | 558 | 77.823 | 10.902 | 10.647 | 1.00 | 27.81 |
| ATOM | 4309 | N | VAL | 559 | 75.601 | 10.870 | 10.313 | 1.00 | 29.20 |
| ATOM | 4311 | CA | VAL | 559 | 75.286 | 10.175 | 11.564 | 1.00 | 29.17 |
| ATOM | 4312 | CB | VAL | 559 | 74.102 | 10.832 | 12.329 | 1.00 | 28.53 |
| ATOM | 4313 | CG1 | VAL | 559 | 73.802 | 10.036 | 13.607 | 1.00 | 27.08 |
| ATOM | 4314 | CG2 | VAL | 559 | 74.456 | 12.281 | 12.687 | 1.00 | 23.27 |
| ATOM | 4315 | C | VAL | 559 | 74.911 | 8.772 | 11.137 | 1.00 | 26.41 |
| ATOM | 4316 | O | VAL | 559 | 73.834 | 8.536 | 10.593 | 1.00 | 25.91 |
| ATOM | 4317 | N | ILE | 560 | 75.824 | 7.846 | 11.371 | 1.00 | 26.71 |
| ATOM | 4319 | CA | ILE | 560 | 75.638 | 6.465 | 10.966 | 1.00 | 27.55 |
| ATOM | 4320 | CB | ILE | 560 | 77.012 | 5.829 | 10.619 | 1.00 | 28.48 |
| ATOM | 4321 | CG2 | ILE | 560 | 76.819 | 4.468 | 9.979 | 1.00 | 29.18 |
| ATOM | 4322 | CG1 | ILE | 560 | 77.793 | 6.745 | 9.657 | 1.00 | 27.99 |
| ATOM | 4323 | CD1 | ILE | 560 | 79.274 | 6.399 | 9.525 | 1.00 | 28.97 |
| ATOM | 4324 | C | ILE | 560 | 74.917 | 5.644 | 12.034 | 1.00 | 29.17 |
| ATOM | 4325 | O | ILE | 560 | 75.404 | 5.497 | 13.160 | 1.00 | 28.92 |
| ATOM | 4326 | N | VAL | 561 | 73.743 | 5.129 | 11.681 | 1.00 | 28.60 |
| ATOM | 4328 | CA | VAL | 561 | 72.957 | 4.325 | 12.606 | 1.00 | 28.58 |
| ATOM | 4329 | CB | VAL | 561 | 71.634 | 5.061 | 13.047 | 1.00 | 27.53 |
| ATOM | 4330 | CG1 | VAL | 561 | 71.951 | 6.400 | 13.701 | 1.00 | 22.44 |
| ATOM | 4331 | CG2 | VAL | 561 | 70.697 | 5.246 | 11.874 | 1.00 | 23.19 |
| ATOM | 4332 | C | VAL | 561 | 72.618 | 2.956 | 12.006 | 1.00 | 28.20 |
| ATOM | 4333 | O | VAL | 561 | 72.875 | 2.694 | 10.825 | 1.00 | 27.99 |
| ATOM | 4334 | N | GLU | 562 | 72.057 | 2.079 | 12.834 | 1.00 | 29.17 |
| ATOM | 4336 | CA | GLU | 562 | 71.666 | 0.744 | 12.399 | 1.00 | 28.96 |
| ATOM | 4337 | CB | GLU | 562 | 71.199 | -0.086 | 13.589 | 1.00 | 27.34 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4338 | CG | GLU | 562 | 72.308 | -0.331 | 14.583 | 1.00 | 30.12 |
| ATOM | 4339 | CD | GLU | 562 | 71.838 | -1.075 | 15.808 | 1.00 | 32.29 |
| ATOM | 4340 | OE1 | GLU | 562 | 72.526 | -2.030 | 16.217 | 1.00 | 32.45 |
| ATOM | 4341 | OE2 | GLU | 562 | 70.785 | -0.702 | 16.362 | 1.00 | 30.16 |
| ATOM | 4342 | C | GLU | 562 | 70.580 | 0.794 | 11.340 | 1.00 | 29.79 |
| ATOM | 4343 | O | GLU | 562 | 69.690 | 1.653 | 11.386 | 1.00 | 29.75 |
| ATOM | 4344 | N | TYR | 563 | 70.684 | -0.106 | 10.369 | 1.00 | 30.51 |
| ATOM | 4346 | CA | TYR | 563 | 69.735 | -0.209 | 9.267 | 1.00 | 33.76 |
| ATOM | 4347 | CB | TYR | 563 | 70.494 | -0.602 | 7.988 | 1.00 | 31.04 |
| ATOM | 4348 | CG | TYR | 563 | 69.624 | -0.928 | 6.806 | 1.00 | 33.40 |
| ATOM | 4349 | CD1 | TYR | 563 | 68.693 | -0.019 | 6.340 | 1.00 | 33.07 |
| ATOM | 4350 | CE1 | TYR | 563 | 67.908 | -0.301 | 5.240 | 1.00 | 34.71 |
| ATOM | 4351 | CD2 | TYR | 563 | 69.749 | -2.141 | 6.147 | 1.00 | 34.61 |
| ATOM | 4352 | CE2 | TYR | 563 | 68.970 | -2.446 | 5.035 | 1.00 | 36.54 |
| ATOM | 4353 | CZ | TYR | 563 | 68.047 | -1.518 | 4.589 | 1.00 | 36.83 |
| ATOM | 4354 | OH | TYR | 563 | 67.261 | -1.805 | 3.501 | 1.00 | 38.81 |
| ATOM | 4356 | C | TYR | 563 | 68.655 | -1.269 | 9.588 | 1.00 | 36.14 |
| ATOM | 4357 | O | TYR | 563 | 68.946 | -2.365 | 10.023 | 1.00 | 37.70 |
| ATOM | 4358 | N | ALA | 564 | 67.406 | -0.948 | 9.309 | 1.00 | 37.87 |
| ATOM | 4360 | CA | ALA | 564 | 66.276 | -1.832 | 9.534 | 1.00 | 38.49 |
| ATOM | 4361 | CB | ALA | 564 | 65.278 | -1.167 | 10.458 | 1.00 | 42.57 |
| ATOM | 4362 | C | ALA | 564 | 65.645 | -2.153 | 8.179 | 1.00 | 39.65 |
| ATOM | 4363 | O | ALA | 564 | 64.796 | -1.423 | 7.687 | 1.00 | 39.74 |
| ATOM | 4364 | N | SER | 565 | 66.039 | -3.280 | 7.607 | 1.00 | 40.06 |
| ATOM | 4366 | CA | SER | 565 | 65.567 | -3.699 | 6.295 | 1.00 | 40.67 |
| ATOM | 4367 | CB | SER | 565 | 66.267 | -4.986 | 5.883 | 1.00 | 38.71 |
| ATOM | 4368 | OG | SER | 565 | 66.107 | -5.964 | 6.889 | 1.00 | 41.35 |
| ATOM | 4370 | C | SER | 565 | 64.081 | -3.884 | 6.106 | 1.00 | 42.17 |
| ATOM | 4371 | O | SER | 565 | 63.585 | -3.741 | 4.992 | 1.00 | 44.25 |
| ATOM | 4372 | N | LYS | 566 | 63.360 | -4.207 | 7.167 | 1.00 | 41.71 |
| ATOM | 4374 | CA | LYS | 566 | 61.928 | -4.427 | 7.015 | 1.00 | 40.22 |
| ATOM | 4375 | CB | LYS | 566 | 61.525 | -5.668 | 7.800 | 1.00 | 39.51 |
| ATOM | 4376 | CG | LYS | 566 | 62.202 | -6.910 | 7.226 | 1.00 | 41.48 |
| ATOM | 4377 | CD | LYS | 566 | 62.113 | -8.094 | 8.149 | 1.00 | 41.53 |
| ATOM | 4378 | CE | LYS | 566 | 62.710 | -9.312 | 7.491 | 1.00 | 41.18 |
| ATOM | 4379 | NZ | LYS | 566 | 62.763 | -10.458 | 8.438 | 1.00 | 46.17 |
| ATOM | 4383 | C | LYS | 566 | 61.007 | -3.220 | 7.263 | 1.00 | 40.47 |
| ATOM | 4384 | O | LYS | 566 | 59.800 | -3.367 | 7.486 | 1.00 | 42.68 |
| ATOM | 4385 | N | GLY | 567 | 61.584 | -2.026 | 7.167 | 1.00 | 38.90 |
| ATOM | 4387 | CA | GLY | 567 | 60.826 | -0.799 | 7.336 | 1.00 | 37.13 |
| ATOM | 4388 | C | GLY | 567 | 60.199 | -0.592 | 8.694 | 1.00 | 36.72 |
| ATOM | 4389 | O | GLY | 567 | 60.644 | -1.172 | 9.683 | 1.00 | 38.48 |
| ATOM | 4390 | N | ASN | 568 | 59.191 | 0.273 | 8.753 | 1.00 | 35.77 |
| ATOM | 4392 | CA | ASN | 568 | 58.518 | 0.549 | 10.015 | 1.00 | 35.36 |
| ATOM | 4393 | CB | ASN | 568 | 57.883 | 1.957 | 10.045 | 1.00 | 36.30 |
| ATOM | 4394 | CG | ASN | 568 | 56.635 | 2.088 | 9.169 | 1.00 | 38.06 |
| ATOM | 4395 | OD1 | ASN | 568 | 55.623 | 1.421 | 9.383 | 1.00 | 38.66 |
| ATOM | 4396 | ND2 | ASN | 568 | 56.686 | 3.010 | 8.221 | 1.00 | 37.29 |
| ATOM | 4399 | C | ASN | 568 | 57.504 | -0.532 | 10.341 | 1.00 | 33.04 |
| ATOM | 4400 | O | ASN | 568 | 57.061 | -1.265 | 9.461 | 1.00 | 32.10 |
| ATOM | 4401 | N | LEU | 569 | 57.142 | -0.612 | 11.617 | 1.00 | 33.59 |
| ATOM | 4403 | CA | LEU | 569 | 56.199 | -1.604 | 12.132 | 1.00 | 32.91 |
| ATOM | 4404 | CB | LEU | 569 | 56.045 | -1.428 | 13.647 | 1.00 | 33.84 |
| ATOM | 4405 | CG | LEU | 569 | 55.088 | -2.343 | 14.403 | 1.00 | 31.96 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4406 | CD1 | LEU | 569 | 55.522 | -3.797 | 14.216 | 1.00 | 33.20 |
| ATOM | 4407 | CD2 | LEU | 569 | 55.089 | -1.967 | 15.868 | 1.00 | 30.81 |
| ATOM | 4408 | C | LEU | 569 | 54.820 | -1.591 | 11.478 | 1.00 | 32.12 |
| ATOM | 4409 | O | LEU | 569 | 54.214 | -2.645 | 11.300 | 1.00 | 33.08 |
| ATOM | 4410 | N | ARG | 570 | 54.315 | -0.409 | 11.148 | 1.00 | 32.05 |
| ATOM | 4412 | CA | ARG | 570 | 52.999 | -0.293 | 10.529 | 1.00 | 35.21 |
| ATOM | 4413 | CB | ARG | 570 | 52.659 | 1.173 | 10.256 | 1.00 | 36.77 |
| ATOM | 4414 | CG | ARG | 570 | 51.282 | 1.370 | 9.653 | 1.00 | 43.11 |
| ATOM | 4415 | CD | ARG | 570 | 51.203 | 2.690 | 8.926 | 1.00 | 49.24 |
| ATOM | 4416 | NE | ARG | 570 | 52.154 | 2.775 | 7.815 | 1.00 | 55.77 |
| ATOM | 4418 | CZ | ARG | 570 | 52.995 | 3.790 | 7.619 | 1.00 | 58.89 |
| ATOM | 4419 | NH1 | ARG | 570 | 53.016 | 4.820 | 8.463 | 1.00 | 61.61 |
| ATOM | 4422 | NH2 | ARG | 570 | 53.804 | 3.786 | 6.566 | 1.00 | 59.16 |
| ATOM | 4425 | C | ARG | 570 | 52.992 | -1.063 | 9.220 | 1.00 | 35.16 |
| ATOM | 4426 | O | ARG | 570 | 52.145 | -1.922 | 8.990 | 1.00 | 35.50 |
| ATOM | 4427 | N | GLU | 571 | 53.971 | -0.760 | 8.383 | 1.00 | 36.29 |
| ATOM | 4429 | CA | GLU | 571 | 54.111 | -1.400 | 7.089 | 1.00 | 37.51 |
| ATOM | 4430 | CB | GLU | 571 | 55.219 | -0.701 | 6.308 | 1.00 | 41.27 |
| ATOM | 4431 | CG | GLU | 571 | 54.945 | 0.778 | 6.110 | 1.00 | 49.88 |
| ATOM | 4432 | CD | GLU | 571 | 56.087 | 1.516 | 5.436 | 1.00 | 57.58 |
| ATOM | 4433 | OE1 | GLU | 571 | 57.264 | 1.122 | 5.636 | 1.00 | 60.59 |
| ATOM | 4434 | OE2 | GLU | 571 | 55.804 | 2.504 | 4.714 | 1.00 | 61.14 |
| ATOM | 4435 | C | GLU | 571 | 54.399 | -2.896 | 7.228 | 1.00 | 36.24 |
| ATOM | 4436 | O | GLU | 571 | 53.889 | -3.716 | 6.459 | 1.00 | 34.22 |
| ATOM | 4437 | N | TYR | 572 | 55.202 | -3.238 | 8.232 | 1.00 | 35.98 |
| ATOM | 4439 | CA | TYR | 572 | 55.570 | -4.619 | 8.517 | 1.00 | 35.34 |
| ATOM | 4440 | CB | TYR | 572 | 56.526 | -4.656 | 9.714 | 1.00 | 30.94 |
| ATOM | 4441 | CG | TYR | 572 | 56.959 | -6.034 | 10.180 | 1.00 | 32.71 |
| ATOM | 4442 | CD1 | TYR | 572 | 58.009 | -6.714 | 9.547 | 1.00 | 32.33 |
| ATOM | 4443 | CE1 | TYR | 572 | 58.464 | -7.940 | 10.026 | 1.00 | 30.31 |
| ATOM | 4444 | CD2 | TYR | 572 | 56.369 | -6.626 | 11.303 | 1.00 | 33.43 |
| ATOM | 4445 | CE2 | TYR | 572 | 56.813 | -7.851 | 11.791 | 1.00 | 31.46 |
| ATOM | 4446 | CZ | TYR | 572 | 57.864 | -8.502 | 11.148 | 1.00 | 33.99 |
| ATOM | 4447 | OH | TYR | 572 | 58.311 | -9.706 | 11.640 | 1.00 | 36.30 |
| ATOM | 4449 | C | TYR | 572 | 54.312 | -5.425 | 8.826 | 1.00 | 37.26 |
| ATOM | 4450 | O | TYR | 572 | 54.121 | -6.530 | 8.314 | 1.00 | 36.91 |
| ATOM | 4451 | N | LEU | 573 | 53.457 | -4.850 | 9.665 | 1.00 | 36.82 |
| ATOM | 4453 | CA | LEU | 573 | 52.208 | -5.476 | 10.075 | 1.00 | 35.56 |
| ATOM | 4454 | CB | LEU | 573 | 51.537 | -4.629 | 11.165 | 1.00 | 34.03 |
| ATOM | 4455 | CG | LEU | 573 | 52.238 | -4.527 | 12.519 | 1.00 | 32.82 |
| ATOM | 4456 | CD1 | LEU | 573 | 51.621 | -3.423 | 13.377 | 1.00 | 28.95 |
| ATOM | 4457 | CD2 | LEU | 573 | 52.168 | -5.858 | 13.207 | 1.00 | 29.46 |
| ATOM | 4458 | C | LEU | 573 | 51.237 | -5.658 | 8.915 | 1.00 | 34.56 |
| ATOM | 4459 | O | LEU | 573 | 50.670 | -6.729 | 8.726 | 1.00 | 34.80 |
| ATOM | 4460 | N | GLN | 574 | 51.030 | -4.602 | 8.150 | 1.00 | 37.10 |
| ATOM | 4462 | CA | GLN | 574 | 50.101 | -4.666 | 7.031 | 1.00 | 41.15 |
| ATOM | 4463 | CB | GLN | 574 | 49.875 | -3.278 | 6.457 | 1.00 | 41.63 |
| ATOM | 4464 | CG | GLN | 574 | 49.089 | -2.375 | 7.366 | 1.00 | 43.13 |
| ATOM | 4465 | CD | GLN | 574 | 49.063 | -0.959 | 6.860 | 1.00 | 47.77 |
| ATOM | 4466 | OE1 | GLN | 574 | 49.655 | -0.647 | 5.827 | 1.00 | 50.00 |
| ATOM | 4467 | NE2 | GLN | 574 | 48.378 | -0.086 | 7.582 | 1.00 | 49.67 |
| ATOM | 4470 | C | GLN | 574 | 50.529 | -5.627 | 5.934 | 1.00 | 42.38 |
| ATOM | 4471 | O | GLN | 574 | 49.685 | -6.284 | 5.318 | 1.00 | 44.56 |
| ATOM | 4472 | N | ALA | 575 | 51.835 | -5.717 | 5.697 | 1.00 | 41.99 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4474 | CA | ALA | 575 | 52.367 | -6.608 | 4.676 | 1.00 | 41.29 |
| ATOM | 4475 | CB | ALA | 575 | 53.841 | -6.325 | 4.446 | 1.00 | 40.43 |
| ATOM | 4476 | C | ALA | 575 | 52.186 | -8.058 | 5.066 | 1.00 | 41.42 |
| ATOM | 4477 | O | ALA | 575 | 52.392 | -8.949 | 4.249 | 1.00 | 43.65 |
| ATOM | 4478 | N | ARG | 576 | 51.815 | -8.294 | 6.319 | 1.00 | 42.56 |
| ATOM | 4480 | CA | ARG | 576 | 51.642 | -9.646 | 6.824 | 1.00 | 42.51 |
| ATOM | 4481 | CB | ARG | 576 | 52.676 | -9.910 | 7.920 | 1.00 | 40.14 |
| ATOM | 4482 | CG | ARG | 576 | 54.100 | -9.896 | 7.377 | 1.00 | 40.32 |
| ATOM | 4483 | CD | ARG | 576 | 55.172 | -9.836 | 8.460 | 1.00 | 40.78 |
| ATOM | 4484 | NE | ARG | 576 | 56.513 | -9.783 | 7.874 | 1.00 | 42.13 |
| ATOM | 4486 | CZ | ARG | 576 | 56.975 | -8.785 | 7.120 | 1.00 | 40.73 |
| ATOM | 4487 | NH1 | ARG | 576 | 56.215 | -7.732 | 6.851 | 1.00 | 39.21 |
| ATOM | 4490 | NH2 | ARG | 576 | 58.201 | -8.846 | 6.622 | 1.00 | 37.62 |
| ATOM | 4493 | C | ARG | 576 | 50.242 | -9.931 | 7.326 | 1.00 | 44.48 |
| ATOM | 4494 | O | ARG | 576 | 50.028 | -10.869 | 8.098 | 1.00 | 46.84 |
| ATOM | 4495 | N | ARG | 577 | 49.275 | -9.146 | 6.866 | 1.00 | 46.26 |
| ATOM | 4497 | CA | ARG | 577 | 47.893 | -9.344 | 7.292 | 1.00 | 46.89 |
| ATOM | 4498 | CB | ARG | 577 | 47.027 | -8.170 | 6.845 | 1.00 | 46.16 |
| ATOM | 4499 | CG | ARG | 577 | 47.189 | -6.939 | 7.696 | 1.00 | 44.93 |
| ATOM | 4500 | CD | ARG | 577 | 46.463 | -5.766 | 7.080 | 1.00 | 44.60 |
| ATOM | 4501 | NE | ARG | 577 | 46.284 | -4.683 | 8.039 | 1.00 | 45.05 |
| ATOM | 4503 | CZ | ARG | 577 | 45.612 | -3.565 | 7.793 | 1.00 | 45.95 |
| ATOM | 4504 | NH1 | ARG | 577 | 45.052 | -3.372 | 6.606 | 1.00 | 47.39 |
| ATOM | 4507 | NH2 | ARG | 577 | 45.466 | -2.655 | 8.749 | 1.00 | 45.49 |
| ATOM | 4510 | C | ARG | 577 | 47.334 | -10.649 | 6.740 | 1.00 | 46.60 |
| ATOM | 4511 | O | ARG | 577 | 47.478 | -10.933 | 5.551 | 1.00 | 47.15 |
| ATOM | 4512 | N | GLN | 594 | 53.312 | -14.007 | 7.967 | 1.00 | 63.97 |
| ATOM | 4514 | CA | GLN | 594 | 52.110 | -14.068 | 8.799 | 1.00 | 63.06 |
| ATOM | 4515 | CB | GLN | 594 | 51.175 | -15.183 | 8.319 | 1.00 | 64.16 |
| ATOM | 4516 | C | GLN | 594 | 52.501 | -14.278 | 10.258 | 1.00 | 61.68 |
| ATOM | 4517 | O | GLN | 594 | 53.101 | -15.292 | 10.619 | 1.00 | 60.95 |
| ATOM | 4518 | N | LEU | 595 | 52.140 | -13.313 | 11.092 | 1.00 | 58.58 |
| ATOM | 4520 | CA | LEU | 595 | 52.470 | -13.335 | 12.505 | 1.00 | 55.58 |
| ATOM | 4521 | CB | LEU | 595 | 52.619 | -11.902 | 13.020 | 1.00 | 54.05 |
| ATOM | 4522 | CG | LEU | 595 | 53.570 | -11.074 | 12.153 | 1.00 | 56.23 |
| ATOM | 4523 | CD1 | LEU | 595 | 53.496 | -9.609 | 12.524 | 1.00 | 58.84 |
| ATOM | 4524 | CD2 | LEU | 595 | 54.977 | -11.596 | 12.301 | 1.00 | 55.93 |
| ATOM | 4525 | C | LEU | 595 | 51.480 | -14.093 | 13.372 | 1.00 | 53.77 |
| ATOM | 4526 | O | LEU | 595 | 50.276 | -14.046 | 13.139 | 1.00 | 54.31 |
| ATOM | 4527 | N | SER | 596 | 52.012 | -14.780 | 14.377 | 1.00 | 51.04 |
| ATOM | 4529 | CA | SER | 596 | 51.206 | -15.541 | 15.316 | 1.00 | 48.97 |
| ATOM | 4530 | CB | SER | 596 | 52.004 | -16.737 | 15.834 | 1.00 | 48.89 |
| ATOM | 4531 | OG | SER | 596 | 52.945 | -16.345 | 16.820 | 1.00 | 48.59 |
| ATOM | 4533 | C | SER | 596 | 50.853 | -14.641 | 16.488 | 1.00 | 47.56 |
| ATOM | 4534 | O | SER | 596 | 51.470 | -13.590 | 16.676 | 1.00 | 46.71 |
| ATOM | 4535 | N | SER | 597 | 49.888 | -15.070 | 17.292 | 1.00 | 47.11 |
| ATOM | 4537 | CA | SER | 597 | 49.462 | -14.315 | 18.461 | 1.00 | 47.88 |
| ATOM | 4538 | CB | SER | 597 | 48.386 | -15.084 | 19.229 | 1.00 | 50.66 |
| ATOM | 4539 | OG | SER | 597 | 47.574 | -15.839 | 18.343 | 1.00 | 57.08 |
| ATOM | 4541 | C | SER | 597 | 50.666 | -14.068 | 19.372 | 1.00 | 46.03 |
| ATOM | 4542 | O | SER | 597 | 50.735 | -13.045 | 20.047 | 1.00 | 46.49 |
| ATOM | 4543 | N | LYS | 598 | 51.607 | -15.007 | 19.399 | 1.00 | 46.08 |
| ATOM | 4545 | CA | LYS | 598 | 52.798 | -14.844 | 20.229 | 1.00 | 46.33 |
| ATOM | 4546 | CB | LYS | 598 | 53.558 | -16.163 | 20.384 | 1.00 | 46.67 |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4547 | CG | LYS | 598 | 54.449 | -16.224 | 21.623 | 1.00 | 49.61 | |
| ATOM | 4548 | CD | LYS | 598 | 55.240 | -17.539 | 21.668 | 1.00 | 53.69 | |
| ATOM | 4549 | CE | LYS | 598 | 55.899 | -17.797 | 23.026 | 1.00 | 53.15 | |
| ATOM | 4550 | NZ | LYS | 598 | 54.891 | -18.076 | 24.093 | 1.00 | 52.02 | |
| ATOM | 4554 | C | LYS | 598 | 53.706 | -13.790 | 19.599 | 1.00 | 45.43 | |
| ATOM | 4555 | O | LYS | 598 | 54.292 | -12.968 | 20.311 | 1.00 | 44.18 | |
| ATOM | 4556 | N | ASP | 599 | 53.780 | -13.804 | 18.264 | 1.00 | 44.16 | |
| ATOM | 4558 | CA | ASP | 599 | 54.598 | -12.851 | 17.513 | 1.00 | 43.46 | |
| ATOM | 4559 | CB | ASP | 599 | 54.523 | -13.098 | 16.001 | 1.00 | 44.83 | |
| ATOM | 4560 | CG | ASP | 599 | 55.288 | -14.336 | 15.560 | 1.00 | 48.24 | |
| ATOM | 4561 | OD1 | ASP | 599 | 56.228 | -14.754 | 16.260 | 1.00 | 52.90 | |
| ATOM | 4562 | OD2 | ASP | 599 | 54.958 | -14.894 | 14.493 | 1.00 | 51.43 | |
| ATOM | 4563 | C | ASP | 599 | 54.120 | -11.437 | 17.796 | 1.00 | 42.71 | |
| ATOM | 4564 | O | ASP | 599 | 54.937 | -10.550 | 18.059 | 1.00 | 45.00 | |
| ATOM | 4565 | N | LEU | 600 | 52.803 | -11.235 | 17.776 | 1.00 | 37.69 | |
| ATOM | 4567 | CA | LEU | 600 | 52.246 | -9.918 | 18.030 | 1.00 | 34.03 | |
| ATOM | 4568 | CB | LEU | 600 | 50.747 | -9.882 | 17.747 | 1.00 | 34.06 | |
| ATOM | 4569 | CG | LEU | 600 | 50.332 | -10.068 | 16.281 | 1.00 | 33.13 | |
| ATOM | 4570 | CD1 | LEU | 600 | 48.814 | -9.992 | 16.190 | 1.00 | 37.38 | |
| ATOM | 4571 | CD2 | LEU | 600 | 50.974 | -9.012 | 15.373 | 1.00 | 25.63 | |
| ATOM | 4572 | C | LEU | 600 | 52.537 | -9.452 | 19.439 | 1.00 | 34.58 | |
| ATOM | 4573 | O | LEU | 600 | 52.910 | -8.294 | 19.636 | 1.00 | 33.18 | |
| ATOM | 4574 | N | VAL | 601 | 52.415 | -10.348 | 20.419 | 1.00 | 34.24 | |
| ATOM | 4576 | CA | VAL | 601 | 52.692 | -9.969 | 21.808 | 1.00 | 35.80 | |
| ATOM | 4577 | CB | VAL | 601 | 52.214 | -11.036 | 22.827 | 1.00 | 37.50 | |
| ATOM | 4578 | CG1 | VAL | 601 | 52.331 | -10.483 | 24.252 | 1.00 | 38.08 | |
| ATOM | 4579 | CG2 | VAL | 601 | 50.766 | -11.409 | 22.560 | 1.00 | 40.77 | |
| ATOM | 4580 | C | VAL | 601 | 54.198 | -9.741 | 21.982 | 1.00 | 35.04 | |
| ATOM | 4581 | O | VAL | 601 | 54.634 | -8.856 | 22.731 | 1.00 | 34.33 | |
| ATOM | 4582 | N | SER | 602 | 54.981 | -10.531 | 21.262 | 1.00 | 32.58 | |
| ATOM | 4584 | CA | SER | 602 | 56.421 | -10.421 | 21.307 | 1.00 | 36.01 | |
| ATOM | 4585 | CB | SER | 602 | 57.045 | -11.504 | 20.439 | 1.00 | 38.43 | |
| ATOM | 4586 | OG | SER | 602 | 58.453 | -11.387 | 20.419 | 1.00 | 43.36 | |
| ATOM | 4588 | C | SER | 602 | 56.809 | -9.038 | 20.800 | 1.00 | 35.21 | |
| ATOM | 4589 | O | SER | 602 | 57.651 | -8.363 | 21.394 | 1.00 | 35.03 | |
| ATOM | 4590 | N | CYS | 603 | 56.183 | -8.614 | 19.707 | 1.00 | 34.15 | |
| ATOM | 4592 | CA | CYS | 603 | 56.438 | -7.294 | 19.141 | 1.00 | 34.04 | |
| ATOM | 4593 | CB | CYS | 603 | 55.543 | -7.055 | 17.925 | 1.00 | 33.45 | |
| ATOM | 4594 | SG | CYS | 603 | 55.653 | -5.423 | 17.229 | 0.50 | 32.19 | PRT1 |
| ATOM | 4595 | C | CYS | 603 | 56.198 | -6.211 | 20.191 | 1.00 | 32.79 | |
| ATOM | 4596 | O | CYS | 603 | 57.023 | -5.316 | 20.362 | 1.00 | 33.36 | |
| ATOM | 4597 | N | ALA | 604 | 55.088 | -6.321 | 20.917 | 1.00 | 31.31 | |
| ATOM | 4599 | CA | ALA | 604 | 54.743 | -5.358 | 21.965 | 1.00 | 32.36 | |
| ATOM | 4600 | CB | ALA | 604 | 53.321 | -5.610 | 22.481 | 1.00 | 32.01 | |
| ATOM | 4601 | C | ALA | 604 | 55.741 | -5.394 | 23.128 | 1.00 | 32.83 | |
| ATOM | 4602 | O | ALA | 604 | 56.050 | -4.358 | 23.727 | 1.00 | 30.89 | |
| ATOM | 4603 | N | TYR | 605 | 56.212 | -6.592 | 23.465 | 1.00 | 32.95 | |
| ATOM | 4605 | CA | TYR | 605 | 57.189 | -6.758 | 24.539 | 1.00 | 33.34 | |
| ATOM | 4606 | CB | TYR | 605 | 57.500 | -8.236 | 24.737 | 1.00 | 32.58 | |
| ATOM | 4607 | CG | TYR | 605 | 58.640 | -8.495 | 25.690 | 1.00 | 32.51 | |
| ATOM | 4608 | CD1 | TYR | 605 | 58.511 | -8.236 | 27.053 | 1.00 | 33.50 | |
| ATOM | 4609 | CE1 | TYR | 605 | 59.556 | -8.507 | 27.943 | 1.00 | 37.08 | |
| ATOM | 4610 | CD2 | TYR | 605 | 59.841 | -9.026 | 25.230 | 1.00 | 34.22 | |
| ATOM | 4611 | CE2 | TYR | 605 | 60.896 | -9.300 | 26.109 | 1.00 | 36.64 | |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4612 | CZ | TYR | 605 | 60.746 | -9.042 | 27.464 | 1.00 | 37.56 |
| ATOM | 4613 | OH | TYR | 605 | 61.776 | -9.342 | 28.336 | 1.00 | 38.08 |
| ATOM | 4615 | C | TYR | 605 | 58.480 | -6.006 | 24.191 | 1.00 | 32.42 |
| ATOM | 4616 | O | TYR | 605 | 58.975 | -5.203 | 24.991 | 1.00 | 33.34 |
| ATOM | 4617 | N | GLN | 606 | 58.997 | -6.267 | 22.989 | 1.00 | 30.61 |
| ATOM | 4619 | CA | GLN | 606 | 60.218 | -5.643 | 22.474 | 1.00 | 31.12 |
| ATOM | 4620 | CB | GLN | 606 | 60.499 | -6.143 | 21.058 | 1.00 | 30.57 |
| ATOM | 4621 | CG | GLN | 606 | 61.044 | -7.568 | 21.008 | 1.00 | 33.90 |
| ATOM | 4622 | CD | GLN | 606 | 61.240 | -8.080 | 19.593 | 1.00 | 32.17 |
| ATOM | 4623 | OE1 | GLN | 606 | 62.155 | -7.652 | 18.883 | 1.00 | 32.55 |
| ATOM | 4624 | NE2 | GLN | 606 | 60.374 | -8.998 | 19.171 | 1.00 | 33.10 |
| ATOM | 4627 | C | GLN | 606 | 60.157 | -4.114 | 22.487 | 1.00 | 31.69 |
| ATOM | 4628 | O | GLN | 606 | 61.111 | -3.453 | 22.910 | 1.00 | 31.18 |
| ATOM | 4629 | N | VAL | 607 | 59.035 | -3.564 | 22.020 | 1.00 | 29.50 |
| ATOM | 4631 | CA | VAL | 607 | 58.816 | -2.122 | 22.000 | 1.00 | 27.54 |
| ATOM | 4632 | CB | VAL | 607 | 57.454 | -1.751 | 21.306 | 1.00 | 26.79 |
| ATOM | 4633 | CG1 | VAL | 607 | 57.131 | -0.291 | 21.516 | 1.00 | 24.80 |
| ATOM | 4634 | CG2 | VAL | 607 | 57.505 | -2.050 | 19.815 | 1.00 | 22.95 |
| ATOM | 4635 | C | VAL | 607 | 58.827 | -1.576 | 23.432 | 1.00 | 28.30 |
| ATOM | 4636 | O | VAL | 607 | 59.469 | -0.548 | 23.705 | 1.00 | 28.32 |
| ATOM | 4637 | N | ALA | 608 | 58.110 | -2.247 | 24.340 | 1.00 | 27.21 |
| ATOM | 4639 | CA | ALA | 608 | 58.061 | -1.805 | 25.735 | 1.00 | 26.54 |
| ATOM | 4640 | CB | ALA | 608 | 57.070 | -2.649 | 26.550 | 1.00 | 26.70 |
| ATOM | 4641 | C | ALA | 608 | 59.457 | -1.850 | 26.368 | 1.00 | 25.97 |
| ATOM | 4642 | O | ALA | 608 | 59.802 | -0.993 | 27.183 | 1.00 | 25.88 |
| ATOM | 4643 | N | ARG | 609 | 60.250 | -2.848 | 25.994 | 1.00 | 26.02 |
| ATOM | 4645 | CA | ARG | 609 | 61.606 | -2.977 | 26.512 | 1.00 | 30.44 |
| ATOM | 4646 | CB | ARG | 609 | 62.234 | -4.285 | 26.058 | 1.00 | 34.09 |
| ATOM | 4647 | CG | ARG | 609 | 61.642 | -5.516 | 26.682 | 1.00 | 39.24 |
| ATOM | 4648 | CD | ARG | 609 | 62.659 | -6.615 | 26.615 | 1.00 | 42.75 |
| ATOM | 4649 | NE | ARG | 609 | 63.405 | -6.704 | 27.860 | 1.00 | 45.52 |
| ATOM | 4651 | CZ | ARG | 609 | 64.525 | -7.405 | 28.019 | 1.00 | 46.24 |
| ATOM | 4652 | NH1 | ARG | 609 | 65.055 | -8.079 | 27.001 | 1.00 | 41.48 |
| ATOM | 4655 | NH2 | ARG | 609 | 65.079 | -7.482 | 29.225 | 1.00 | 47.49 |
| ATOM | 4658 | C | ARG | 609 | 62.478 | -1.829 | 26.015 | 1.00 | 34.20 |
| ATOM | 4659 | O | ARG | 609 | 63.265 | -1.255 | 26.788 | 1.00 | 35.24 |
| ATOM | 4660 | N | GLY | 610 | 62.368 | -1.528 | 24.717 | 1.00 | 33.25 |
| ATOM | 4662 | CA | GLY | 610 | 63.130 | -0.439 | 24.138 | 1.00 | 29.57 |
| ATOM | 4663 | C | GLY | 610 | 62.802 | 0.814 | 24.908 | 1.00 | 29.31 |
| ATOM | 4664 | O | GLY | 610 | 63.695 | 1.543 | 25.335 | 1.00 | 27.46 |
| ATOM | 4665 | N | MET | 611 | 61.507 | 1.020 | 25.147 | 1.00 | 31.07 |
| ATOM | 4667 | CA | MET | 611 | 61.016 | 2.178 | 25.889 | 1.00 | 30.09 |
| ATOM | 4668 | CB | MET | 611 | 59.493 | 2.280 | 25.782 | 1.00 | 29.51 |
| ATOM | 4669 | CG | MET | 611 | 58.997 | 2.655 | 24.404 | 1.00 | 28.21 |
| ATOM | 4670 | SD | MET | 611 | 59.760 | 4.175 | 23.787 | 1.00 | 29.00 |
| ATOM | 4671 | CE | MET | 611 | 59.350 | 5.335 | 25.039 | 1.00 | 25.91 |
| ATOM | 4672 | C | MET | 611 | 61.439 | 2.189 | 27.361 | 1.00 | 30.47 |
| ATOM | 4673 | O | MET | 611 | 61.734 | 3.242 | 27.919 | 1.00 | 29.43 |
| ATOM | 4674 | N | GLU | 612 | 61.429 | 1.031 | 28.002 | 1.00 | 31.97 |
| ATOM | 4676 | CA | GLU | 612 | 61.836 | 0.947 | 29.402 | 1.00 | 35.34 |
| ATOM | 4677 | CB | GLU | 612 | 61.707 | -0.490 | 29.904 | 1.00 | 36.17 |
| ATOM | 4678 | CG | GLU | 612 | 62.305 | -0.729 | 31.278 | 1.00 | 34.87 |
| ATOM | 4679 | CD | GLU | 612 | 62.259 | -2.185 | 31.705 | 1.00 | 32.68 |
| ATOM | 4680 | OE1 | GLU | 612 | 62.641 | -3.070 | 30.904 | 1.00 | 35.01 |

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|---|---|---|---|---|---|---|---|---|
| ATOM | 4681 | OE2 | GLU | 612 | 61.848 | -2.443 | 32.858 | 1.00 | 36.56 |
| ATOM | 4682 | C | GLU | 612 | 63.296 | 1.425 | 29.490 | 1.00 | 35.26 |
| ATOM | 4683 | O | GLU | 612 | 63.677 | 2.162 | 30.417 | 1.00 | 31.21 |
| ATOM | 4684 | N | TYR | 613 | 64.092 | 1.040 | 28.491 | 1.00 | 36.10 |
| ATOM | 4686 | CA | TYR | 613 | 65.491 | 1.458 | 28.440 | 1.00 | 34.76 |
| ATOM | 4687 | CB | TYR | 613 | 66.249 | 0.788 | 27.301 | 1.00 | 31.15 |
| ATOM | 4688 | CG | TYR | 613 | 67.700 | 1.195 | 27.284 | 1.00 | 34.28 |
| ATOM | 4689 | CD1 | TYR | 613 | 68.600 | 0.654 | 28.207 | 1.00 | 36.50 |
| ATOM | 4690 | CE1 | TYR | 613 | 69.949 | 1.035 | 28.219 | 1.00 | 38.20 |
| ATOM | 4691 | CD2 | TYR | 613 | 68.179 | 2.135 | 26.366 | 1.00 | 32.99 |
| ATOM | 4692 | CE2 | TYR | 613 | 69.520 | 2.526 | 26.372 | 1.00 | 33.32 |
| ATOM | 4693 | CZ | TYR | 613 | 70.399 | 1.968 | 27.302 | 1.00 | 36.59 |
| ATOM | 4694 | OH | TYR | 613 | 71.721 | 2.340 | 27.333 | 1.00 | 35.73 |
| ATOM | 4696 | C | TYR | 613 | 65.583 | 2.970 | 28.273 | 1.00 | 34.03 |
| ATOM | 4697 | O | TYR | 613 | 66.231 | 3.643 | 29.075 | 1.00 | 35.26 |
| ATOM | 4698 | N | LEU | 614 | 64.916 | 3.503 | 27.250 | 1.00 | 31.78 |
| ATOM | 4700 | CA | LEU | 614 | 64.945 | 4.937 | 26.998 | 1.00 | 29.50 |
| ATOM | 4701 | CB | LEU | 614 | 64.095 | 5.297 | 25.775 | 1.00 | 28.26 |
| ATOM | 4702 | CG | LEU | 614 | 64.564 | 4.742 | 24.422 | 1.00 | 31.29 |
| ATOM | 4703 | CD1 | LEU | 614 | 63.564 | 5.089 | 23.321 | 1.00 | 28.09 |
| ATOM | 4704 | CD2 | LEU | 614 | 65.951 | 5.282 | 24.079 | 1.00 | 29.52 |
| ATOM | 4705 | C | LEU | 614 | 64.489 | 5.715 | 28.224 | 1.00 | 32.49 |
| ATOM | 4706 | O | LEU | 614 | 65.108 | 6.717 | 28.598 | 1.00 | 31.73 |
| ATOM | 4707 | N | ALA | 615 | 63.431 | 5.232 | 28.872 | 1.00 | 33.06 |
| ATOM | 4709 | CA | ALA | 615 | 62.906 | 5.870 | 30.070 | 1.00 | 35.16 |
| ATOM | 4710 | CB | ALA | 615 | 61.598 | 5.192 | 30.511 | 1.00 | 36.64 |
| ATOM | 4711 | C | ALA | 615 | 63.942 | 5.838 | 31.202 | 1.00 | 35.36 |
| ATOM | 4712 | O | ALA | 615 | 64.065 | 6.805 | 31.952 | 1.00 | 36.80 |
| ATOM | 4713 | N | SER | 616 | 64.690 | 4.739 | 31.315 | 1.00 | 35.91 |
| ATOM | 4715 | CA | SER | 616 | 65.716 | 4.621 | 32.354 | 1.00 | 35.78 |
| ATOM | 4716 | CB | SER | 616 | 66.287 | 3.199 | 32.424 | 1.00 | 32.52 |
| ATOM | 4717 | OG | SER | 616 | 67.133 | 2.899 | 31.324 | 1.00 | 29.64 |
| ATOM | 4719 | C | SER | 616 | 66.832 | 5.623 | 32.063 | 1.00 | 37.48 |
| ATOM | 4720 | O | SER | 616 | 67.556 | 6.048 | 32.967 | 1.00 | 38.76 |
| ATOM | 4721 | N | LYS | 617 | 66.971 | 5.980 | 30.790 | 1.00 | 34.74 |
| ATOM | 4723 | CA | LYS | 617 | 67.973 | 6.931 | 30.357 | 1.00 | 32.44 |
| ATOM | 4724 | CB | LYS | 617 | 68.540 | 6.520 | 28.998 | 1.00 | 32.94 |
| ATOM | 4725 | CG | LYS | 617 | 69.330 | 5.232 | 29.041 | 1.00 | 32.64 |
| ATOM | 4726 | CD | LYS | 617 | 70.539 | 5.402 | 29.933 | 1.00 | 38.45 |
| ATOM | 4727 | CE | LYS | 617 | 71.252 | 4.091 | 30.139 | 1.00 | 40.84 |
| ATOM | 4728 | NZ | LYS | 617 | 72.552 | 4.306 | 30.812 | 1.00 | 46.49 |
| ATOM | 4732 | C | LYS | 617 | 67.376 | 8.325 | 30.281 | 1.00 | 33.29 |
| ATOM | 4733 | O | LYS | 617 | 67.909 | 9.188 | 29.598 | 1.00 | 33.95 |
| ATOM | 4734 | N | LYS | 618 | 66.245 | 8.528 | 30.952 | 1.00 | 34.87 |
| ATOM | 4736 | CA | LYS | 618 | 65.569 | 9.822 | 30.997 | 1.00 | 35.44 |
| ATOM | 4737 | CB | LYS | 618 | 66.512 | 10.868 | 31.581 | 1.00 | 40.44 |
| ATOM | 4738 | CG | LYS | 618 | 67.192 | 10.446 | 32.877 | 1.00 | 48.19 |
| ATOM | 4739 | CD | LYS | 618 | 66.234 | 10.363 | 34.037 | 1.00 | 55.47 |
| ATOM | 4740 | CE | LYS | 618 | 66.962 | 9.939 | 35.310 | 1.00 | 61.56 |
| ATOM | 4741 | NZ | LYS | 618 | 66.070 | 10.032 | 36.514 | 1.00 | 68.82 |
| ATOM | 4745 | C | LYS | 618 | 65.015 | 10.327 | 29.663 | 1.00 | 35.62 |
| ATOM | 4746 | O | LYS | 618 | 64.557 | 11.463 | 29.569 | 1.00 | 36.44 |
| ATOM | 4747 | N | CYS | 619 | 65.006 | 9.472 | 28.647 | 1.00 | 34.24 |
| ATOM | 4749 | CA | CYS | 619 | 64.525 | 9.848 | 27.323 | 1.00 | 31.62 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4750 | CB | CYS | 619 | 65.279 | 9.033 | 26.263 | 1.00 | 31.17 |
| ATOM | 4751 | SG | CYS | 619 | 64.816 | 9.306 | 24.541 | 1.00 | 30.02 |
| ATOM | 4752 | C | CYS | 619 | 63.004 | 9.701 | 27.149 | 1.00 | 30.45 |
| ATOM | 4753 | O | CYS | 619 | 62.418 | 8.649 | 27.388 | 1.00 | 29.24 |
| ATOM | 4754 | N | ILE | 620 | 62.359 | 10.798 | 26.800 | 1.00 | 30.14 |
| ATOM | 4756 | CA | ILE | 620 | 60.935 | 10.822 | 26.542 | 1.00 | 31.76 |
| ATOM | 4757 | CB | ILE | 620 | 60.268 | 12.040 | 27.193 | 1.00 | 31.26 |
| ATOM | 4758 | CG2 | ILE | 620 | 58.799 | 12.116 | 26.774 | 1.00 | 31.66 |
| ATOM | 4759 | CG1 | ILE | 620 | 60.392 | 11.957 | 28.712 | 1.00 | 29.71 |
| ATOM | 4760 | CD1 | ILE | 620 | 60.016 | 13.236 | 29.396 | 1.00 | 27.40 |
| ATOM | 4761 | C | ILE | 620 | 60.864 | 10.961 | 25.023 | 1.00 | 31.86 |
| ATOM | 4762 | O | ILE | 620 | 61.384 | 11.920 | 24.465 | 1.00 | 32.70 |
| ATOM | 4763 | N | HIS | 621 | 60.249 | 9.986 | 24.366 | 1.00 | 31.70 |
| ATOM | 4765 | CA | HIS | 621 | 60.133 | 9.973 | 22.906 | 1.00 | 32.12 |
| ATOM | 4766 | CB | HIS | 621 | 59.708 | 8.578 | 22.430 | 1.00 | 29.61 |
| ATOM | 4767 | CG | HIS | 621 | 59.903 | 8.344 | 20.961 | 1.00 | 28.62 |
| ATOM | 4768 | CD2 | HIS | 621 | 60.511 | 7.336 | 20.300 | 1.00 | 27.49 |
| ATOM | 4769 | ND1 | HIS | 621 | 59.373 | 9.168 | 19.988 | 1.00 | 30.08 |
| ATOM | 4771 | CE1 | HIS | 621 | 59.637 | 8.669 | 18.795 | 1.00 | 25.00 |
| ATOM | 4772 | NE2 | HIS | 621 | 60.325 | 7.554 | 18.956 | 1.00 | 26.55 |
| ATOM | 4774 | C | HIS | 621 | 59.194 | 11.026 | 22.321 | 1.00 | 34.51 |
| ATOM | 4775 | O | HIS | 621 | 59.466 | 11.570 | 21.251 | 1.00 | 36.79 |
| ATOM | 4776 | N | ARG | 622 | 58.048 | 11.248 | 22.960 | 1.00 | 35.26 |
| ATOM | 4778 | CA | ARG | 622 | 57.068 | 12.239 | 22.490 | 1.00 | 34.68 |
| ATOM | 4779 | CB | ARG | 622 | 57.705 | 13.628 | 22.370 | 1.00 | 33.43 |
| ATOM | 4780 | CG | ARG | 622 | 58.285 | 14.135 | 23.674 | 1.00 | 31.52 |
| ATOM | 4781 | CD | ARG | 622 | 58.781 | 15.563 | 23.570 | 0.50 | 27.82 |
| ATOM | 4782 | NE | ARG | 622 | 59.216 | 16.050 | 24.876 | 0.50 | 28.82 |
| ATOM | 4784 | CZ | ARG | 622 | 60.362 | 15.715 | 25.463 | 0.50 | 30.41 |
| ATOM | 4785 | NH1 | ARG | 622 | 61.215 | 14.891 | 24.860 | 0.50 | 31.15 |
| ATOM | 4788 | NH2 | ARG | 622 | 60.640 | 16.168 | 26.680 | 0.50 | 30.83 |
| ATOM | 4791 | C | ARG | 622 | 56.283 | 11.891 | 21.213 | 1.00 | 34.71 |
| ATOM | 4792 | O | ARG | 622 | 55.289 | 12.544 | 20.912 | 1.00 | 35.58 |
| ATOM | 4793 | N | ASP | 623 | 56.719 | 10.884 | 20.459 | 1.00 | 34.90 |
| ATOM | 4795 | CA | ASP | 623 | 55.986 | 10.468 | 19.261 | 1.00 | 34.30 |
| ATOM | 4796 | CB | ASP | 623 | 56.443 | 11.212 | 17.994 | 1.00 | 36.76 |
| ATOM | 4797 | CG | ASP | 623 | 55.535 | 10.918 | 16.772 | 1.00 | 43.35 |
| ATOM | 4798 | OD1 | ASP | 623 | 55.980 | 11.131 | 15.624 | 1.00 | 47.64 |
| ATOM | 4799 | OD2 | ASP | 623 | 54.376 | 10.469 | 16.954 | 1.00 | 43.30 |
| ATOM | 4800 | C | ASP | 623 | 56.094 | 8.967 | 19.051 | 1.00 | 32.24 |
| ATOM | 4801 | O | ASP | 623 | 56.406 | 8.494 | 17.957 | 1.00 | 31.19 |
| ATOM | 4802 | N | LEU | 624 | 55.895 | 8.209 | 20.118 | 1.00 | 32.27 |
| ATOM | 4804 | CA | LEU | 624 | 55.964 | 6.759 | 20.005 | 1.00 | 33.18 |
| ATOM | 4805 | CB | LEU | 624 | 56.013 | 6.118 | 21.390 | 1.00 | 31.16 |
| ATOM | 4806 | CG | LEU | 624 | 56.019 | 4.592 | 21.452 | 1.00 | 32.74 |
| ATOM | 4807 | CD1 | LEU | 624 | 57.257 | 4.020 | 20.765 | 1.00 | 30.64 |
| ATOM | 4808 | CD2 | LEU | 624 | 55.974 | 4.177 | 22.904 | 1.00 | 34.51 |
| ATOM | 4809 | C | LEU | 624 | 54.738 | 6.274 | 19.217 | 1.00 | 35.18 |
| ATOM | 4810 | O | LEU | 624 | 53.589 | 6.511 | 19.612 | 1.00 | 35.72 |
| ATOM | 4811 | N | ALA | 625 | 54.997 | 5.632 | 18.084 | 1.00 | 32.37 |
| ATOM | 4813 | CA | ALA | 625 | 53.946 | 5.113 | 17.223 | 1.00 | 30.60 |
| ATOM | 4814 | CB | ALA | 625 | 53.447 | 6.205 | 16.298 | 1.00 | 25.26 |
| ATOM | 4815 | C | ALA | 625 | 54.618 | 4.020 | 16.427 | 1.00 | 29.87 |
| ATOM | 4816 | O | ALA | 625 | 55.839 | 3.978 | 16.378 | 1.00 | 32.01 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4817 | N | ALA | 626 | 53.834 | 3.163 | 15.779 | 1.00 | 30.12 |
| ATOM | 4819 | CA | ALA | 626 | 54.373 | 2.057 | 14.978 | 1.00 | 29.62 |
| ATOM | 4820 | CB | ALA | 626 | 53.231 | 1.159 | 14.441 | 1.00 | 27.11 |
| ATOM | 4821 | C | ALA | 626 | 55.255 | 2.552 | 13.838 | 1.00 | 26.57 |
| ATOM | 4822 | O | ALA | 626 | 56.193 | 1.871 | 13.434 | 1.00 | 26.29 |
| ATOM | 4823 | N | ARG | 627 | 54.935 | 3.730 | 13.317 | 1.00 | 26.74 |
| ATOM | 4825 | CA | ARG | 627 | 55.706 | 4.352 | 12.244 | 1.00 | 28.73 |
| ATOM | 4826 | CB | ARG | 627 | 55.056 | 5.671 | 11.827 | 1.00 | 29.62 |
| ATOM | 4827 | CG | ARG | 627 | 54.894 | 6.659 | 12.972 | 1.00 | 31.84 |
| ATOM | 4828 | CD | ARG | 627 | 54.435 | 8.032 | 12.485 | 1.00 | 38.54 |
| ATOM | 4829 | NE | ARG | 627 | 53.987 | 8.878 | 13.590 | 1.00 | 38.59 |
| ATOM | 4831 | CZ | ARG | 627 | 52.745 | 8.879 | 14.064 | 1.00 | 39.55 |
| ATOM | 4832 | NH1 | ARG | 627 | 51.822 | 8.094 | 13.525 | 1.00 | 35.96 |
| ATOM | 4835 | NH2 | ARG | 627 | 52.447 | 9.604 | 15.127 | 1.00 | 41.05 |
| ATOM | 4838 | C | ARG | 627 | 57.151 | 4.632 | 12.676 | 1.00 | 30.79 |
| ATOM | 4839 | O | ARG | 627 | 58.058 | 4.687 | 11.838 | 1.00 | 30.16 |
| ATOM | 4840 | N | ASN | 628 | 57.347 | 4.822 | 13.985 | 1.00 | 30.31 |
| ATOM | 4842 | CA | ASN | 628 | 58.661 | 5.109 | 14.550 | 1.00 | 28.50 |
| ATOM | 4843 | CB | ASN | 628 | 58.587 | 6.257 | 15.549 | 1.00 | 27.84 |
| ATOM | 4844 | CG | ASN | 628 | 58.369 | 7.571 | 14.868 | 1.00 | 31.41 |
| ATOM | 4845 | OD1 | ASN | 628 | 58.893 | 7.796 | 13.782 | 1.00 | 33.45 |
| ATOM | 4846 | ND2 | ASN | 628 | 57.551 | 8.429 | 15.460 | 1.00 | 28.53 |
| ATOM | 4849 | C | ASN | 628 | 59.352 | 3.919 | 15.169 | 1.00 | 28.10 |
| ATOM | 4850 | O | ASN | 628 | 60.232 | 4.076 | 16.021 | 1.00 | 28.64 |
| ATOM | 4851 | N | VAL | 629 | 58.887 | 2.733 | 14.803 | 1.00 | 27.79 |
| ATOM | 4853 | CA | VAL | 629 | 59.484 | 1.482 | 15.253 | 1.00 | 28.30 |
| ATOM | 4854 | CB | VAL | 629 | 58.475 | 0.577 | 15.983 | 1.00 | 25.38 |
| ATOM | 4855 | CG1 | VAL | 629 | 59.118 | -0.753 | 16.284 | 1.00 | 23.07 |
| ATOM | 4856 | CG2 | VAL | 629 | 57.980 | 1.246 | 17.265 | 1.00 | 22.48 |
| ATOM | 4857 | C | VAL | 629 | 59.925 | 0.810 | 13.949 | 1.00 | 28.69 |
| ATOM | 4858 | O | VAL | 629 | 59.114 | 0.616 | 13.043 | 1.00 | 27.07 |
| ATOM | 4859 | N | LEU | 630 | 61.220 | 0.542 | 13.823 | 1.00 | 29.54 |
| ATOM | 4861 | CA | LEU | 630 | 61.749 | -0.081 | 12.616 | 1.00 | 30.17 |
| ATOM | 4862 | CB | LEU | 630 | 62.999 | 0.659 | 12.142 | 1.00 | 29.62 |
| ATOM | 4863 | CG | LEU | 630 | 62.831 | 2.180 | 12.035 | 1.00 | 29.14 |
| ATOM | 4864 | CD1 | LEU | 630 | 64.121 | 2.795 | 11.579 | 1.00 | 29.83 |
| ATOM | 4865 | CD2 | LEU | 630 | 61.693 | 2.543 | 11.086 | 1.00 | 32.59 |
| ATOM | 4866 | C | LEU | 630 | 62.036 | -1.541 | 12.899 | 1.00 | 30.50 |
| ATOM | 4867 | O | LEU | 630 | 62.290 | -1.910 | 14.042 | 1.00 | 31.06 |
| ATOM | 4868 | N | VAL | 631 | 61.966 | -2.376 | 11.866 | 1.00 | 33.03 |
| ATOM | 4870 | CA | VAL | 631 | 62.174 | -3.813 | 12.022 | 1.00 | 31.83 |
| ATOM | 4871 | CB | VAL | 631 | 60.902 | -4.605 | 11.582 | 1.00 | 29.48 |
| ATOM | 4872 | CG1 | VAL | 631 | 61.017 | -6.067 | 11.980 | 1.00 | 29.39 |
| ATOM | 4873 | CG2 | VAL | 631 | 59.644 | -3.984 | 12.196 | 1.00 | 25.38 |
| ATOM | 4874 | C | VAL | 631 | 63.379 | -4.242 | 11.196 | 1.00 | 32.37 |
| ATOM | 4875 | O | VAL | 631 | 63.508 | -3.865 | 10.024 | 1.00 | 33.57 |
| ATOM | 4876 | N | THR | 632 | 64.285 | -4.987 | 11.820 | 1.00 | 34.39 |
| ATOM | 4878 | CA | THR | 632 | 65.504 | -5.453 | 11.145 | 1.00 | 35.84 |
| ATOM | 4879 | CB | THR | 632 | 66.659 | -5.685 | 12.148 | 1.00 | 33.11 |
| ATOM | 4880 | OG1 | THR | 632 | 66.328 | -6.774 | 13.020 | 1.00 | 34.88 |
| ATOM | 4882 | CG2 | THR | 632 | 66.922 | -4.426 | 12.972 | 1.00 | 28.85 |
| ATOM | 4883 | C | THR | 632 | 65.272 | -6.738 | 10.350 | 1.00 | 37.63 |
| ATOM | 4884 | O | THR | 632 | 64.195 | -7.347 | 10.439 | 1.00 | 37.20 |
| ATOM | 4885 | N | GLU | 633 | 66.289 | -7.163 | 9.600 | 1.00 | 39.78 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4887 | CA | GLU | 633 | 66.182 | -8.379 | 8.794 | 1.00 | 43.30 |
| ATOM | 4888 | CB | GLU | 633 | 67.437 | -8.590 | 7.933 | 1.00 | 46.66 |
| ATOM | 4889 | CG | GLU | 633 | 67.336 | -9.729 | 6.876 | 1.00 | 51.37 |
| ATOM | 4890 | CD | GLU | 633 | 66.490 | -9.404 | 5.622 | 1.00 | 54.30 |
| ATOM | 4891 | OE1 | GLU | 633 | 65.859 | -8.327 | 5.523 | 1.00 | 55.85 |
| ATOM | 4892 | OE2 | GLU | 633 | 66.460 | -10.256 | 4.710 | 1.00 | 55.95 |
| ATOM | 4893 | C | GLU | 633 | 65.919 | -9.592 | 9.677 | 1.00 | 42.72 |
| ATOM | 4894 | O | GLU | 633 | 65.360 | -10.582 | 9.222 | 1.00 | 45.10 |
| ATOM | 4895 | N | ASP | 634 | 66.287 | -9.494 | 10.949 | 1.00 | 42.83 |
| ATOM | 4897 | CA | ASP | 634 | 66.075 | -10.585 | 11.884 | 1.00 | 43.03 |
| ATOM | 4898 | CB | ASP | 634 | 67.324 | -10.809 | 12.743 | 1.00 | 49.02 |
| ATOM | 4899 | CG | ASP | 634 | 68.539 | -11.240 | 11.916 | 1.00 | 55.95 |
| ATOM | 4900 | OD1 | ASP | 634 | 68.462 | -12.292 | 11.237 | 1.00 | 59.10 |
| ATOM | 4901 | OD2 | ASP | 634 | 69.568 | -10.525 | 11.943 | 1.00 | 59.41 |
| ATOM | 4902 | C | ASP | 634 | 64.848 | -10.340 | 12.751 | 1.00 | 41.75 |
| ATOM | 4903 | O | ASP | 634 | 64.737 | -10.873 | 13.847 | 1.00 | 42.79 |
| ATOM | 4904 | N | ASN | 635 | 63.937 | -9.508 | 12.257 | 1.00 | 42.51 |
| ATOM | 4906 | CA | ASN | 635 | 62.686 | -9.186 | 12.939 | 1.00 | 42.53 |
| ATOM | 4907 | CB | ASN | 635 | 61.768 | -10.417 | 12.992 | 1.00 | 45.07 |
| ATOM | 4908 | CG | ASN | 635 | 61.483 | -10.985 | 11.624 | 1.00 | 46.54 |
| ATOM | 4909 | OD1 | ASN | 635 | 60.868 | -10.336 | 10.786 | 1.00 | 49.77 |
| ATOM | 4910 | ND2 | ASN | 635 | 61.949 | -12.192 | 11.383 | 1.00 | 49.29 |
| ATOM | 4913 | C | ASN | 635 | 62.801 | -8.577 | 14.331 | 1.00 | 40.51 |
| ATOM | 4914 | O | ASN | 635 | 61.939 | -8.800 | 15.187 | 1.00 | 41.80 |
| ATOM | 4915 | N | VAL | 636 | 63.844 | -7.795 | 14.561 | 1.00 | 37.98 |
| ATOM | 4917 | CA | VAL | 636 | 64.016 | -7.164 | 15.856 | 1.00 | 33.92 |
| ATOM | 4918 | CB | VAL | 636 | 65.517 | -7.005 | 16.195 | 1.00 | 32.21 |
| ATOM | 4919 | CG1 | VAL | 636 | 65.697 | -6.284 | 17.530 | 1.00 | 31.40 |
| ATOM | 4920 | CG2 | VAL | 636 | 66.169 | -8.367 | 16.242 | 1.00 | 30.93 |
| ATOM | 4921 | C | VAL | 636 | 63.349 | -5.797 | 15.811 | 1.00 | 31.85 |
| ATOM | 4922 | O | VAL | 636 | 63.531 | -5.061 | 14.849 | 1.00 | 33.47 |
| ATOM | 4923 | N | MET | 637 | 62.525 | -5.492 | 16.807 | 1.00 | 31.69 |
| ATOM | 4925 | CA | MET | 637 | 61.860 | -4.194 | 16.879 | 1.00 | 31.44 |
| ATOM | 4926 | CB | MET | 637 | 60.642 | -4.241 | 17.820 | 1.00 | 34.97 |
| ATOM | 4927 | CG | MET | 637 | 59.559 | -5.264 | 17.455 | 1.00 | 36.80 |
| ATOM | 4928 | SD | MET | 637 | 58.860 | -5.048 | 15.803 | 1.00 | 35.45 |
| ATOM | 4929 | CE | MET | 637 | 59.030 | -6.709 | 15.116 | 1.00 | 32.12 |
| ATOM | 4930 | C | MET | 637 | 62.874 | -3.209 | 17.454 | 1.00 | 31.86 |
| ATOM | 4931 | O | MET | 637 | 63.512 | -3.496 | 18.479 | 1.00 | 29.47 |
| ATOM | 4932 | N | LYS | 638 | 62.985 | -2.041 | 16.820 | 1.00 | 30.87 |
| ATOM | 4934 | CA | LYS | 638 | 63.915 | -0.994 | 17.244 | 1.00 | 29.66 |
| ATOM | 4935 | CB | LYS | 638 | 65.161 | -0.983 | 16.349 | 1.00 | 27.51 |
| ATOM | 4936 | CG | LYS | 638 | 66.171 | -2.059 | 16.691 | 1.00 | 27.29 |
| ATOM | 4937 | CD | LYS | 638 | 67.370 | -1.984 | 15.781 | 1.00 | 28.55 |
| ATOM | 4938 | CE | LYS | 638 | 68.409 | -3.029 | 16.150 | 1.00 | 24.75 |
| ATOM | 4939 | NZ | LYS | 638 | 68.964 | -2.785 | 17.498 | 1.00 | 25.59 |
| ATOM | 4943 | C | LYS | 638 | 63.283 | 0.383 | 17.215 | 1.00 | 27.72 |
| ATOM | 4944 | O | LYS | 638 | 62.918 | 0.869 | 16.146 | 1.00 | 27.66 |
| ATOM | 4945 | N | ILE | 639 | 63.163 | 1.004 | 18.387 | 1.00 | 26.21 |
| ATOM | 4947 | CA | ILE | 639 | 62.597 | 2.343 | 18.501 | 1.00 | 26.27 |
| ATOM | 4948 | CB | ILE | 639 | 62.580 | 2.862 | 19.965 | 1.00 | 26.52 |
| ATOM | 4949 | CG2 | ILE | 639 | 61.896 | 4.206 | 20.017 | 1.00 | 21.50 |
| ATOM | 4950 | CG1 | ILE | 639 | 61.918 | 1.854 | 20.926 | 1.00 | 25.70 |
| ATOM | 4951 | CD1 | ILE | 639 | 60.496 | 1.494 | 20.599 | 1.00 | 25.62 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4952 | C | ILE | 639 | 63.505 | 3.288 | 17.718 | 1.00 | 29.56 |
| ATOM | 4953 | O | ILE | 639 | 64.730 | 3.281 | 17.906 | 1.00 | 27.74 |
| ATOM | 4954 | N | ALA | 640 | 62.897 | 4.101 | 16.857 | 1.00 | 27.91 |
| ATOM | 4956 | CA | ALA | 640 | 63.620 | 5.071 | 16.042 | 1.00 | 28.79 |
| ATOM | 4957 | CB | ALA | 640 | 63.377 | 4.796 | 14.563 | 1.00 | 26.74 |
| ATOM | 4958 | C | ALA | 640 | 63.164 | 6.487 | 16.385 | 1.00 | 28.91 |
| ATOM | 4959 | O | ALA | 640 | 62.087 | 6.683 | 16.956 | 1.00 | 28.67 |
| ATOM | 4960 | N | ASP | 641 | 64.007 | 7.464 | 16.067 | 1.00 | 28.25 |
| ATOM | 4962 | CA | ASP | 641 | 63.708 | 8.876 | 16.296 | 1.00 | 30.80 |
| ATOM | 4963 | CB | ASP | 641 | 62.520 | 9.319 | 15.428 | 1.00 | 33.44 |
| ATOM | 4964 | CG | ASP | 641 | 62.869 | 9.393 | 13.948 | 1.00 | 38.01 |
| ATOM | 4965 | OD1 | ASP | 641 | 64.002 | 9.001 | 13.574 | 1.00 | 42.41 |
| ATOM | 4966 | OD2 | ASP | 641 | 62.006 | 9.847 | 13.160 | 1.00 | 41.74 |
| ATOM | 4967 | C | ASP | 641 | 63.501 | 9.311 | 17.745 | 1.00 | 29.07 |
| ATOM | 4968 | O | ASP | 641 | 62.847 | 10.309 | 18.020 | 1.00 | 28.42 |
| ATOM | 4969 | N | PHE | 642 | 64.138 | 8.604 | 18.663 | 1.00 | 29.69 |
| ATOM | 4971 | CA | PHE | 642 | 64.036 | 8.914 | 20.074 | 1.00 | 29.62 |
| ATOM | 4972 | CB | PHE | 642 | 64.347 | 7.656 | 20.890 | 1.00 | 27.18 |
| ATOM | 4973 | CG | PHE | 642 | 65.702 | 7.058 | 20.603 | 1.00 | 23.96 |
| ATOM | 4974 | CD1 | PHE | 642 | 66.848 | 7.559 | 21.219 | 1.00 | 23.66 |
| ATOM | 4975 | CD2 | PHE | 642 | 65.828 | 5.974 | 19.742 | 1.00 | 24.08 |
| ATOM | 4976 | CE1 | PHE | 642 | 68.090 | 6.992 | 20.980 | 1.00 | 23.02 |
| ATOM | 4977 | CE2 | PHE | 642 | 67.069 | 5.403 | 19.501 | 1.00 | 23.20 |
| ATOM | 4978 | CZ | PHE | 642 | 68.200 | 5.909 | 20.121 | 1.00 | 21.68 |
| ATOM | 4979 | C | PHE | 642 | 64.948 | 10.075 | 20.502 | 1.00 | 32.99 |
| ATOM | 4980 | O | PHE | 642 | 64.755 | 10.664 | 21.574 | 1.00 | 32.10 |
| ATOM | 4981 | N | GLY | 643 | 65.940 | 10.396 | 19.671 | 1.00 | 34.66 |
| ATOM | 4983 | CA | GLY | 643 | 66.869 | 11.463 | 20.003 | 1.00 | 35.29 |
| ATOM | 4984 | C | GLY | 643 | 66.639 | 12.755 | 19.250 | 1.00 | 39.13 |
| ATOM | 4985 | O | GLY | 643 | 67.464 | 13.666 | 19.333 | 1.00 | 39.83 |
| ATOM | 4986 | N | LEU | 644 | 65.520 | 12.850 | 18.532 | 1.00 | 42.26 |
| ATOM | 4988 | CA | LEU | 644 | 65.202 | 14.043 | 17.745 | 1.00 | 46.25 |
| ATOM | 4989 | CB | LEU | 644 | 63.935 | 13.843 | 16.911 | 1.00 | 44.59 |
| ATOM | 4990 | CG | LEU | 644 | 63.911 | 12.839 | 15.763 | 1.00 | 43.00 |
| ATOM | 4991 | CD1 | LEU | 644 | 62.653 | 13.068 | 14.940 | 1.00 | 42.61 |
| ATOM | 4992 | CD2 | LEU | 644 | 65.119 | 13.016 | 14.889 | 1.00 | 45.65 |
| ATOM | 4993 | C | LEU | 644 | 65.037 | 15.298 | 18.578 | 1.00 | 49.59 |
| ATOM | 4994 | O | LEU | 644 | 64.391 | 15.281 | 19.623 | 1.00 | 51.90 |
| ATOM | 4995 | N | ALA | 645 | 65.585 | 16.401 | 18.080 | 1.00 | 52.08 |
| ATOM | 4997 | CA | ALA | 645 | 65.495 | 17.677 | 18.777 | 1.00 | 54.71 |
| ATOM | 4998 | CB | ALA | 645 | 66.414 | 18.699 | 18.124 | 1.00 | 54.38 |
| ATOM | 4999 | C | ALA | 645 | 64.053 | 18.184 | 18.790 | 1.00 | 55.44 |
| ATOM | 5000 | O | ALA | 645 | 63.534 | 18.582 | 19.832 | 1.00 | 56.69 |
| ATOM | 5001 | N | ASP | 652 | 52.389 | 21.543 | 14.759 | 1.00 | 73.74 |
| ATOM | 5003 | CA | ASP | 652 | 51.207 | 21.745 | 13.934 | 1.00 | 73.83 |
| ATOM | 5004 | CB | ASP | 652 | 51.601 | 21.995 | 12.472 | 1.00 | 73.22 |
| ATOM | 5005 | CG | ASP | 652 | 50.398 | 22.241 | 11.569 | 1.00 | 72.95 |
| ATOM | 5006 | OD1 | ASP | 652 | 49.354 | 22.715 | 12.065 | 1.00 | 73.71 |
| ATOM | 5007 | OD2 | ASP | 652 | 50.497 | 21.956 | 10.357 | 1.00 | 73.02 |
| ATOM | 5008 | C | ASP | 652 | 50.321 | 20.514 | 14.042 | 1.00 | 75.11 |
| ATOM | 5009 | O | ASP | 652 | 50.568 | 19.495 | 13.394 | 1.00 | 75.96 |
| ATOM | 5010 | N | TYR | 653 | 49.272 | 20.628 | 14.849 | 1.00 | 75.57 |
| ATOM | 5012 | CA | TYR | 653 | 48.348 | 19.524 | 15.064 | 1.00 | 75.68 |
| ATOM | 5013 | CB | TYR | 653 | 47.274 | 19.914 | 16.088 | 1.00 | 76.85 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5014 | CG | TYR | 653 | 47.771 | 19.995 | 17.519 | 1.00 | 79.55 |
| ATOM | 5015 | CD1 | TYR | 653 | 46.983 | 20.567 | 18.518 | 1.00 | 80.89 |
| ATOM | 5016 | CE1 | TYR | 653 | 47.438 | 20.648 | 19.836 | 1.00 | 83.02 |
| ATOM | 5017 | CD2 | TYR | 653 | 49.032 | 19.503 | 17.874 | 1.00 | 80.87 |
| ATOM | 5018 | CE2 | TYR | 653 | 49.496 | 19.578 | 19.183 | 1.00 | 81.70 |
| ATOM | 5019 | CZ | TYR | 653 | 48.698 | 20.152 | 20.160 | 1.00 | 83.09 |
| ATOM | 5020 | OH | TYR | 653 | 49.165 | 20.243 | 21.451 | 1.00 | 83.73 |
| ATOM | 5022 | C | TYR | 653 | 47.685 | 19.038 | 13.787 | 1.00 | 75.03 |
| ATOM | 5023 | O | TYR | 653 | 47.232 | 17.897 | 13.711 | 1.00 | 75.97 |
| ATOM | 5024 | N | TYR | 654 | 47.679 | 19.885 | 12.767 | 1.00 | 73.85 |
| ATOM | 5026 | CA | TYR | 654 | 47.039 | 19.538 | 11.507 | 1.00 | 73.32 |
| ATOM | 5027 | CB | TYR | 654 | 46.276 | 20.750 | 10.972 | 1.00 | 71.97 |
| ATOM | 5028 | CG | TYR | 654 | 45.259 | 21.276 | 11.954 | 1.00 | 70.94 |
| ATOM | 5029 | CD1 | TYR | 654 | 45.659 | 21.801 | 13.185 | 1.00 | 71.41 |
| ATOM | 5030 | CE1 | TYR | 654 | 44.733 | 22.234 | 14.121 | 1.00 | 73.60 |
| ATOM | 5031 | CD2 | TYR | 654 | 43.899 | 21.206 | 11.680 | 1.00 | 71.81 |
| ATOM | 5032 | CE2 | TYR | 654 | 42.956 | 21.642 | 12.610 | 1.00 | 74.81 |
| ATOM | 5033 | CZ | TYR | 654 | 43.380 | 22.152 | 13.832 | 1.00 | 74.84 |
| ATOM | 5034 | OH | TYR | 654 | 42.457 | 22.571 | 14.769 | 1.00 | 76.60 |
| ATOM | 5036 | C | TYR | 654 | 47.975 | 18.967 | 10.446 | 1.00 | 73.82 |
| ATOM | 5037 | O | TYR | 654 | 47.545 | 18.671 | 9.329 | 1.00 | 74.25 |
| ATOM | 5038 | N | LYS | 655 | 49.249 | 18.806 | 10.784 | 1.00 | 74.04 |
| ATOM | 5040 | CA | LYS | 655 | 50.195 | 18.256 | 9.827 | 1.00 | 75.41 |
| ATOM | 5041 | CB | LYS | 655 | 51.626 | 18.680 | 10.164 | 1.00 | 78.45 |
| ATOM | 5042 | CG | LYS | 655 | 52.647 | 18.198 | 9.151 | 1.00 | 83.01 |
| ATOM | 5043 | CD | LYS | 655 | 54.062 | 18.589 | 9.537 | 1.00 | 87.72 |
| ATOM | 5044 | CE | LYS | 655 | 55.076 | 17.813 | 8.703 | 1.00 | 91.45 |
| ATOM | 5045 | NZ | LYS | 655 | 56.489 | 18.133 | 9.074 | 1.00 | 94.17 |
| ATOM | 5049 | C | LYS | 655 | 50.075 | 16.736 | 9.832 | 1.00 | 75.50 |
| ATOM | 5050 | O | LYS | 655 | 50.245 | 16.092 | 10.872 | 1.00 | 75.90 |
| ATOM | 5051 | N | LYS | 656 | 49.750 | 16.173 | 8.672 | 1.00 | 75.26 |
| ATOM | 5053 | CA | LYS | 656 | 49.597 | 14.730 | 8.533 | 1.00 | 74.97 |
| ATOM | 5054 | CB | LYS | 656 | 48.723 | 14.406 | 7.323 | 1.00 | 75.40 |
| ATOM | 5055 | CG | LYS | 656 | 47.266 | 14.753 | 7.519 | 1.00 | 76.87 |
| ATOM | 5056 | CD | LYS | 656 | 46.489 | 14.535 | 6.239 | 1.00 | 80.75 |
| ATOM | 5057 | CE | LYS | 656 | 45.001 | 14.655 | 6.483 | 1.00 | 83.60 |
| ATOM | 5058 | NZ | LYS | 656 | 44.236 | 14.637 | 5.204 | 1.00 | 87.14 |
| ATOM | 5062 | C | LYS | 656 | 50.939 | 14.016 | 8.414 | 1.00 | 74.58 |
| ATOM | 5063 | O | LYS | 656 | 51.904 | 14.578 | 7.897 | 1.00 | 75.01 |
| ATOM | 5064 | N | GLY | 660 | 49.137 | 9.764 | 5.736 | 1.00 | 59.18 |
| ATOM | 5066 | CA | GLY | 660 | 48.106 | 10.781 | 5.848 | 1.00 | 56.19 |
| ATOM | 5067 | C | GLY | 660 | 47.407 | 10.761 | 7.192 | 1.00 | 55.31 |
| ATOM | 5068 | O | GLY | 660 | 46.289 | 11.263 | 7.328 | 1.00 | 56.96 |
| ATOM | 5069 | N | ARG | 661 | 48.059 | 10.163 | 8.183 | 1.00 | 53.02 |
| ATOM | 5071 | CA | ARG | 661 | 47.493 | 10.083 | 9.527 | 1.00 | 49.80 |
| ATOM | 5072 | CB | ARG | 661 | 47.944 | 8.799 | 10.229 | 1.00 | 51.79 |
| ATOM | 5073 | CG | ARG | 661 | 47.683 | 7.523 | 9.450 | 1.00 | 50.59 |
| ATOM | 5074 | CD | ARG | 661 | 47.822 | 6.323 | 10.367 | 1.00 | 53.68 |
| ATOM | 5075 | NE | ARG | 661 | 47.714 | 5.044 | 9.665 | 1.00 | 52.66 |
| ATOM | 5077 | CZ | ARG | 661 | 47.928 | 3.863 | 10.236 | 1.00 | 51.73 |
| ATOM | 5078 | NH1 | ARG | 661 | 48.264 | 3.794 | 11.518 | 1.00 | 50.23 |
| ATOM | 5081 | NH2 | ARG | 661 | 47.800 | 2.751 | 9.528 | 1.00 | 52.58 |
| ATOM | 5084 | C | ARG | 661 | 47.915 | 11.297 | 10.346 | 1.00 | 44.80 |
| ATOM | 5085 | O | ARG | 661 | 48.865 | 11.998 | 9.986 | 1.00 | 43.61 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5086 | N | LEU | 662 | 47.221 | 11.528 | 11.453 | 1.00 | 40.74 |
| ATOM | 5088 | CA | LEU | 662 | 47.518 | 12.654 | 12.333 | 1.00 | 37.88 |
| ATOM | 5089 | CB | LEU | 662 | 46.234 | 13.415 | 12.671 | 1.00 | 36.19 |
| ATOM | 5090 | CG | LEU | 662 | 45.515 | 14.074 | 11.499 | 1.00 | 35.32 |
| ATOM | 5091 | CD1 | LEU | 662 | 44.045 | 14.278 | 11.831 | 1.00 | 31.05 |
| ATOM | 5092 | CD2 | LEU | 662 | 46.217 | 15.383 | 11.156 | 1.00 | 34.37 |
| ATOM | 5093 | C | LEU | 662 | 48.162 | 12.170 | 13.622 | 1.00 | 35.34 |
| ATOM | 5094 | O | LEU | 662 | 47.529 | 11.479 | 14.417 | 1.00 | 33.06 |
| ATOM | 5095 | N | PRO | 663 | 49.441 | 12.518 | 13.843 | 1.00 | 36.39 |
| ATOM | 5096 | CD | PRO | 663 | 50.375 | 13.113 | 12.868 | 1.00 | 37.57 |
| ATOM | 5097 | CA | PRO | 663 | 50.158 | 12.107 | 15.054 | 1.00 | 36.39 |
| ATOM | 5098 | CB | PRO | 663 | 51.516 | 12.787 | 14.885 | 1.00 | 36.98 |
| ATOM | 5099 | CG | PRO | 663 | 51.728 | 12.657 | 13.401 | 1.00 | 38.48 |
| ATOM | 5100 | C | PRO | 663 | 49.477 | 12.491 | 16.371 | 1.00 | 35.47 |
| ATOM | 5101 | O | PRO | 663 | 49.699 | 11.841 | 17.392 | 1.00 | 35.08 |
| ATOM | 5102 | N | VAL | 664 | 48.646 | 13.532 | 16.362 | 1.00 | 34.28 |
| ATOM | 5104 | CA | VAL | 664 | 47.951 | 13.931 | 17.583 | 1.00 | 34.43 |
| ATOM | 5105 | CB | VAL | 664 | 47.038 | 15.181 | 17.376 | 1.00 | 36.92 |
| ATOM | 5106 | CG1 | VAL | 664 | 47.885 | 16.408 | 17.160 | 1.00 | 37.55 |
| ATOM | 5107 | CG2 | VAL | 664 | 46.091 | 14.989 | 16.186 | 1.00 | 38.28 |
| ATOM | 5108 | C | VAL | 664 | 47.137 | 12.749 | 18.120 | 1.00 | 33.03 |
| ATOM | 5109 | O | VAL | 664 | 46.908 | 12.641 | 19.318 | 1.00 | 34.62 |
| ATOM | 5110 | N | LYS | 665 | 46.803 | 11.809 | 17.236 | 1.00 | 32.47 |
| ATOM | 5112 | CA | LYS | 665 | 46.040 | 10.631 | 17.614 | 1.00 | 30.71 |
| ATOM | 5113 | CB | LYS | 665 | 45.456 | 9.958 | 16.370 | 1.00 | 29.59 |
| ATOM | 5114 | CG | LYS | 665 | 44.324 | 10.774 | 15.768 | 1.00 | 29.64 |
| ATOM | 5115 | CD | LYS | 665 | 43.927 | 10.334 | 14.367 | 1.00 | 31.86 |
| ATOM | 5116 | CE | LYS | 665 | 42.664 | 11.056 | 13.899 | 1.00 | 30.42 |
| ATOM | 5117 | NZ | LYS | 665 | 42.296 | 10.720 | 12.486 | 1.00 | 26.50 |
| ATOM | 5121 | C | LYS | 665 | 46.801 | 9.644 | 18.498 | 1.00 | 32.23 |
| ATOM | 5122 | O | LYS | 665 | 46.230 | 8.659 | 18.955 | 1.00 | 30.04 |
| ATOM | 5123 | N | TRP | 666 | 48.080 | 9.915 | 18.748 | 1.00 | 31.38 |
| ATOM | 5125 | CA | TRP | 666 | 48.886 | 9.068 | 19.619 | 1.00 | 32.32 |
| ATOM | 5126 | CB | TRP | 666 | 50.204 | 8.682 | 18.945 | 1.00 | 31.07 |
| ATOM | 5127 | CG | TRP | 666 | 50.078 | 7.530 | 18.006 | 1.00 | 28.26 |
| ATOM | 5128 | CD2 | TRP | 666 | 49.531 | 7.559 | 16.684 | 1.00 | 27.07 |
| ATOM | 5129 | CE2 | TRP | 666 | 49.630 | 6.257 | 16.163 | 1.00 | 26.71 |
| ATOM | 5130 | CE3 | TRP | 666 | 48.982 | 8.569 | 15.882 | 1.00 | 26.56 |
| ATOM | 5131 | CD1 | TRP | 666 | 50.473 | 6.238 | 18.234 | 1.00 | 24.97 |
| ATOM | 5132 | NE1 | TRP | 666 | 50.206 | 5.469 | 17.132 | 1.00 | 27.38 |
| ATOM | 5134 | CZ2 | TRP | 666 | 49.190 | 5.929 | 14.874 | 1.00 | 27.22 |
| ATOM | 5135 | CZ3 | TRP | 666 | 48.548 | 8.248 | 14.599 | 1.00 | 30.14 |
| ATOM | 5136 | CH2 | TRP | 666 | 48.658 | 6.934 | 14.107 | 1.00 | 26.64 |
| ATOM | 5137 | C | TRP | 666 | 49.203 | 9.802 | 20.913 | 1.00 | 33.84 |
| ATOM | 5138 | O | TRP | 666 | 49.688 | 9.202 | 21.873 | 1.00 | 32.82 |
| ATOM | 5139 | N | MET | 667 | 48.905 | 11.099 | 20.929 | 1.00 | 35.75 |
| ATOM | 5141 | CA | MET | 667 | 49.180 | 11.960 | 22.069 | 1.00 | 37.60 |
| ATOM | 5142 | CB | MET | 667 | 49.150 | 13.423 | 21.641 | 1.00 | 41.95 |
| ATOM | 5143 | CG | MET | 667 | 50.487 | 13.975 | 21.226 | 1.00 | 48.44 |
| ATOM | 5144 | SD | MET | 667 | 50.384 | 15.728 | 20.919 | 1.00 | 55.33 |
| ATOM | 5145 | CE | MET | 667 | 50.711 | 15.745 | 19.183 | 1.00 | 49.29 |
| ATOM | 5146 | C | MET | 667 | 48.294 | 11.802 | 23.289 | 1.00 | 38.98 |
| ATOM | 5147 | O | MET | 667 | 47.066 | 11.699 | 23.183 | 1.00 | 39.18 |
| ATOM | 5148 | N | ALA | 668 | 48.933 | 11.824 | 24.456 | 1.00 | 38.72 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5150 | CA | ALA | 668 | 48.231 | 11.728 | 25.727 | 1.00 | 37.82 |
| ATOM | 5151 | CB | ALA | 668 | 49.224 | 11.527 | 26.857 | 1.00 | 38.49 |
| ATOM | 5152 | C | ALA | 668 | 47.497 | 13.051 | 25.891 | 1.00 | 38.16 |
| ATOM | 5153 | O | ALA | 668 | 47.937 | 14.072 | 25.363 | 1.00 | 37.21 |
| ATOM | 5154 | N | PRO | 669 | 46.383 | 13.062 | 26.644 | 1.00 | 39.78 |
| ATOM | 5155 | CD | PRO | 669 | 45.785 | 11.931 | 27.367 | 1.00 | 40.08 |
| ATOM | 5156 | CA | PRO | 669 | 45.598 | 14.281 | 26.858 | 1.00 | 40.68 |
| ATOM | 5157 | CB | PRO | 669 | 44.474 | 13.806 | 27.782 | 1.00 | 42.15 |
| ATOM | 5158 | CG | PRO | 669 | 44.346 | 12.352 | 27.446 | 1.00 | 42.56 |
| ATOM | 5159 | C | PRO | 669 | 46.398 | 15.432 | 27.484 | 1.00 | 42.69 |
| ATOM | 5160 | O | PRO | 669 | 46.320 | 16.566 | 27.019 | 1.00 | 42.14 |
| ATOM | 5161 | N | GLU | 670 | 47.168 | 15.153 | 28.532 | 1.00 | 43.21 |
| ATOM | 5163 | CA | GLU | 670 | 47.956 | 16.211 | 29.160 | 1.00 | 44.62 |
| ATOM | 5164 | CB | GLU | 670 | 48.651 | 15.719 | 30.429 | 1.00 | 44.95 |
| ATOM | 5165 | CG | GLU | 670 | 49.824 | 14.782 | 30.197 | 1.00 | 45.54 |
| ATOM | 5166 | CD | GLU | 670 | 49.422 | 13.332 | 30.079 | 1.00 | 42.72 |
| ATOM | 5167 | OE1 | GLU | 670 | 50.332 | 12.481 | 30.066 | 1.00 | 41.43 |
| ATOM | 5168 | OE2 | GLU | 670 | 48.212 | 13.036 | 30.015 | 1.00 | 44.44 |
| ATOM | 5169 | C | GLU | 670 | 48.993 | 16.772 | 28.195 | 1.00 | 44.88 |
| ATOM | 5170 | O | GLU | 670 | 49.248 | 17.968 | 28.194 | 1.00 | 45.08 |
| ATOM | 5171 | N | ALA | 671 | 49.565 | 15.908 | 27.358 | 1.00 | 44.75 |
| ATOM | 5173 | CA | ALA | 671 | 50.573 | 16.323 | 26.392 | 1.00 | 45.92 |
| ATOM | 5174 | CB | ALA | 671 | 51.256 | 15.095 | 25.766 | 1.00 | 44.10 |
| ATOM | 5175 | C | ALA | 671 | 49.944 | 17.193 | 25.314 | 1.00 | 47.96 |
| ATOM | 5176 | O | ALA | 671 | 50.526 | 18.192 | 24.894 | 1.00 | 49.16 |
| ATOM | 5177 | N | LEU | 672 | 48.729 | 16.836 | 24.917 | 1.00 | 49.84 |
| ATOM | 5179 | CA | LEU | 672 | 47.989 | 17.554 | 23.881 | 1.00 | 50.74 |
| ATOM | 5180 | CB | LEU | 672 | 46.926 | 16.619 | 23.289 | 1.00 | 53.20 |
| ATOM | 5181 | CG | LEU | 672 | 46.184 | 16.989 | 22.004 | 1.00 | 55.26 |
| ATOM | 5182 | CD1 | LEU | 672 | 47.153 | 17.155 | 20.856 | 1.00 | 57.12 |
| ATOM | 5183 | CD2 | LEU | 672 | 45.203 | 15.895 | 21.680 | 1.00 | 52.86 |
| ATOM | 5184 | C | LEU | 672 | 47.327 | 18.826 | 24.408 | 1.00 | 50.79 |
| ATOM | 5185 | O | LEU | 672 | 47.302 | 19.855 | 23.736 | 1.00 | 50.95 |
| ATOM | 5186 | N | PHE | 673 | 46.792 | 18.751 | 25.618 | 1.00 | 52.07 |
| ATOM | 5188 | CA | PHE | 673 | 46.111 | 19.884 | 26.226 | 1.00 | 54.39 |
| ATOM | 5189 | CB | PHE | 673 | 44.892 | 19.396 | 27.019 | 1.00 | 51.21 |
| ATOM | 5190 | CG | PHE | 673 | 43.871 | 18.656 | 26.186 | 1.00 | 48.49 |
| ATOM | 5191 | CD1 | PHE | 673 | 43.304 | 17.473 | 26.646 | 1.00 | 47.79 |
| ATOM | 5192 | CD2 | PHE | 673 | 43.470 | 19.149 | 24.949 | 1.00 | 49.04 |
| ATOM | 5193 | CE1 | PHE | 673 | 42.349 | 16.789 | 25.888 | 1.00 | 47.90 |
| ATOM | 5194 | CE2 | PHE | 673 | 42.511 | 18.473 | 24.182 | 1.00 | 49.71 |
| ATOM | 5195 | CZ | PHE | 673 | 41.952 | 17.288 | 24.655 | 1.00 | 46.86 |
| ATOM | 5196 | C | PHE | 673 | 47.007 | 20.741 | 27.123 | 1.00 | 58.25 |
| ATOM | 5197 | O | PHE | 673 | 47.000 | 21.971 | 27.034 | 1.00 | 60.52 |
| ATOM | 5198 | N | ASP | 674 | 47.784 | 20.094 | 27.983 | 1.00 | 59.63 |
| ATOM | 5200 | CA | ASP | 674 | 48.652 | 20.815 | 28.905 | 1.00 | 62.11 |
| ATOM | 5201 | CB | ASP | 674 | 48.568 | 20.196 | 30.307 | 1.00 | 63.81 |
| ATOM | 5202 | CG | ASP | 674 | 47.143 | 20.015 | 30.791 | 1.00 | 66.46 |
| ATOM | 5203 | OD1 | ASP | 674 | 46.815 | 18.901 | 31.247 | 1.00 | 66.70 |
| ATOM | 5204 | OD2 | ASP | 674 | 46.354 | 20.981 | 30.722 | 1.00 | 68.77 |
| ATOM | 5205 | C | ASP | 674 | 50.119 | 20.852 | 28.482 | 1.00 | 63.36 |
| ATOM | 5206 | O | ASP | 674 | 50.979 | 21.175 | 29.310 | 1.00 | 64.11 |
| ATOM | 5207 | N | ARG | 675 | 50.410 | 20.486 | 27.228 | 1.00 | 62.94 |
| ATOM | 5209 | CA | ARG | 675 | 51.789 | 20.456 | 26.706 | 1.00 | 60.75 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5210 | CB | ARG | 675 | 52.277 | 21.874 | 26.360 | 1.00 | 60.56 |
| ATOM | 5211 | CG | ARG | 675 | 51.474 | 22.560 | 25.261 | 1.00 | 63.67 |
| ATOM | 5212 | CD | ARG | 675 | 51.986 | 23.970 | 24.964 | 1.00 | 66.99 |
| ATOM | 5213 | NE | ARG | 675 | 53.308 | 23.980 | 24.337 | 1.00 | 69.34 |
| ATOM | 5215 | CZ | ARG | 675 | 54.063 | 25.068 | 24.173 | 1.00 | 68.48 |
| ATOM | 5216 | NH1 | ARG | 675 | 53.637 | 26.254 | 24.590 | 1.00 | 65.81 |
| ATOM | 5219 | NH2 | ARG | 675 | 55.254 | 24.965 | 23.593 | 1.00 | 68.76 |
| ATOM | 5222 | C | ARG | 675 | 52.750 | 19.793 | 27.700 | 1.00 | 58.06 |
| ATOM | 5223 | O | ARG | 675 | 53.933 | 20.130 | 27.766 | 1.00 | 59.30 |
| ATOM | 5224 | N | ILE | 676 | 52.221 | 18.859 | 28.483 | 1.00 | 55.62 |
| ATOM | 5226 | CA | ILE | 676 | 52.992 | 18.141 | 29.489 | 1.00 | 54.09 |
| ATOM | 5227 | CB | ILE | 676 | 52.154 | 17.921 | 30.765 | 1.00 | 52.69 |
| ATOM | 5228 | CG2 | ILE | 676 | 52.749 | 16.811 | 31.629 | 1.00 | 49.38 |
| ATOM | 5229 | CG1 | ILE | 676 | 52.049 | 19.230 | 31.540 | 1.00 | 53.15 |
| ATOM | 5230 | CD1 | ILE | 676 | 51.306 | 19.103 | 32.845 | 1.00 | 57.79 |
| ATOM | 5231 | C | ILE | 676 | 53.468 | 16.796 | 28.953 | 1.00 | 53.83 |
| ATOM | 5232 | O | ILE | 676 | 52.668 | 15.891 | 28.730 | 1.00 | 54.87 |
| ATOM | 5233 | N | TYR | 677 | 54.773 | 16.671 | 28.745 | 1.00 | 51.76 |
| ATOM | 5235 | CA | TYR | 677 | 55.343 | 15.436 | 28.236 | 1.00 | 49.42 |
| ATOM | 5236 | CB | TYR | 677 | 56.232 | 15.722 | 27.031 | 1.00 | 51.33 |
| ATOM | 5237 | CG | TYR | 677 | 55.466 | 16.181 | 25.809 | 1.00 | 56.22 |
| ATOM | 5238 | CD1 | TYR | 677 | 55.158 | 17.529 | 25.619 | 1.00 | 56.12 |
| ATOM | 5239 | CE1 | TYR | 677 | 54.491 | 17.960 | 24.479 | 1.00 | 56.18 |
| ATOM | 5240 | CD2 | TYR | 677 | 55.078 | 15.269 | 24.823 | 1.00 | 58.13 |
| ATOM | 5241 | CE2 | TYR | 677 | 54.411 | 15.689 | 23.679 | 1.00 | 57.65 |
| ATOM | 5242 | CZ | TYR | 677 | 54.125 | 17.035 | 23.512 | 1.00 | 58.23 |
| ATOM | 5243 | OH | TYR | 677 | 53.504 | 17.457 | 22.360 | 1.00 | 61.71 |
| ATOM | 5245 | C | TYR | 677 | 56.136 | 14.730 | 29.316 | 1.00 | 46.46 |
| ATOM | 5246 | O | TYR | 677 | 56.983 | 15.335 | 29.970 | 1.00 | 48.65 |
| ATOM | 5247 | N | THR | 678 | 55.818 | 13.464 | 29.537 | 1.00 | 41.73 |
| ATOM | 5249 | CA | THR | 678 | 56.498 | 12.664 | 30.535 | 1.00 | 39.83 |
| ATOM | 5250 | CB | THR | 678 | 55.680 | 12.593 | 31.861 | 1.00 | 41.78 |
| ATOM | 5251 | OG1 | THR | 678 | 54.462 | 11.867 | 31.642 | 1.00 | 45.77 |
| ATOM | 5253 | CG2 | THR | 678 | 55.342 | 13.988 | 32.383 | 1.00 | 41.84 |
| ATOM | 5254 | C | THR | 678 | 56.661 | 11.242 | 30.011 | 1.00 | 37.46 |
| ATOM | 5255 | O | THR | 678 | 56.258 | 10.917 | 28.897 | 1.00 | 37.51 |
| ATOM | 5256 | N | HIS | 679 | 57.264 | 10.388 | 30.825 | 1.00 | 36.36 |
| ATOM | 5258 | CA | HIS | 679 | 57.423 | 9.003 | 30.457 | 1.00 | 35.91 |
| ATOM | 5259 | CB | HIS | 679 | 58.348 | 8.294 | 31.439 | 1.00 | 35.05 |
| ATOM | 5260 | CG | HIS | 679 | 59.761 | 8.798 | 31.404 | 1.00 | 37.68 |
| ATOM | 5261 | CD2 | HIS | 679 | 60.453 | 9.569 | 32.278 | 1.00 | 37.89 |
| ATOM | 5262 | ND1 | HIS | 679 | 60.632 | 8.507 | 30.380 | 1.00 | 37.49 |
| ATOM | 5264 | CE1 | HIS | 679 | 61.803 | 9.071 | 30.621 | 1.00 | 39.58 |
| ATOM | 5265 | NE2 | HIS | 679 | 61.721 | 9.722 | 31.766 | 1.00 | 39.81 |
| ATOM | 5267 | C | HIS | 679 | 56.032 | 8.376 | 30.441 | 1.00 | 36.76 |
| ATOM | 5268 | O | HIS | 679 | 55.771 | 7.458 | 29.660 | 1.00 | 37.16 |
| ATOM | 5269 | N | GLN | 680 | 55.126 | 8.908 | 31.264 | 1.00 | 36.27 |
| ATOM | 5271 | CA | GLN | 680 | 53.754 | 8.407 | 31.332 | 1.00 | 37.71 |
| ATOM | 5272 | CB | GLN | 680 | 53.069 | 8.815 | 32.640 | 1.00 | 40.95 |
| ATOM | 5273 | CG | GLN | 680 | 53.645 | 8.128 | 33.884 | 1.00 | 45.23 |
| ATOM | 5274 | CD | GLN | 680 | 53.676 | 6.595 | 33.780 | 1.00 | 44.44 |
| ATOM | 5275 | OE1 | GLN | 680 | 52.669 | 5.925 | 33.996 | 1.00 | 42.76 |
| ATOM | 5276 | NE2 | GLN | 680 | 54.846 | 6.043 | 33.464 | 1.00 | 40.57 |
| ATOM | 5279 | C | GLN | 680 | 52.927 | 8.842 | 30.121 | 1.00 | 37.54 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5280 | O | GLN | 680 | 51.950 | 8.185 | 29.765 | 1.00 | 37.93 |
| ATOM | 5281 | N | SER | 681 | 53.282 | 9.961 | 29.504 | 1.00 | 36.38 |
| ATOM | 5283 | CA | SER | 681 | 52.563 | 10.367 | 28.306 | 1.00 | 38.05 |
| ATOM | 5284 | CB | SER | 681 | 52.857 | 11.819 | 27.940 | 1.00 | 41.41 |
| ATOM | 5285 | OG | SER | 681 | 54.239 | 12.069 | 27.938 | 1.00 | 42.92 |
| ATOM | 5287 | C | SER | 681 | 52.991 | 9.421 | 27.178 | 1.00 | 37.92 |
| ATOM | 5288 | O | SER | 681 | 52.205 | 9.148 | 26.263 | 1.00 | 37.21 |
| ATOM | 5289 | N | ASP | 682 | 54.237 | 8.932 | 27.248 | 1.00 | 34.77 |
| ATOM | 5291 | CA | ASP | 682 | 54.750 | 7.972 | 26.267 | 1.00 | 31.99 |
| ATOM | 5292 | CB | ASP | 682 | 56.243 | 7.683 | 26.481 | 1.00 | 31.08 |
| ATOM | 5293 | CG | ASP | 682 | 57.165 | 8.638 | 25.721 | 1.00 | 33.63 |
| ATOM | 5294 | OD1 | ASP | 682 | 58.386 | 8.503 | 25.920 | 1.00 | 32.35 |
| ATOM | 5295 | OD2 | ASP | 682 | 56.707 | 9.500 | 24.930 | 1.00 | 29.46 |
| ATOM | 5296 | C | ASP | 682 | 53.969 | 6.672 | 26.457 | 1.00 | 31.54 |
| ATOM | 5297 | O | ASP | 682 | 53.675 | 5.971 | 25.493 | 1.00 | 29.94 |
| ATOM | 5298 | N | VAL | 683 | 53.677 | 6.334 | 27.712 | 1.00 | 30.48 |
| ATOM | 5300 | CA | VAL | 683 | 52.913 | 5.126 | 28.023 | 1.00 | 32.94 |
| ATOM | 5301 | CB | VAL | 683 | 52.731 | 4.939 | 29.572 | 1.00 | 33.94 |
| ATOM | 5302 | CG1 | VAL | 683 | 51.635 | 3.905 | 29.872 | 1.00 | 32.71 |
| ATOM | 5303 | CG2 | VAL | 683 | 54.042 | 4.474 | 30.209 | 1.00 | 27.41 |
| ATOM | 5304 | C | VAL | 683 | 51.545 | 5.164 | 27.299 | 1.00 | 32.27 |
| ATOM | 5305 | O | VAL | 683 | 51.106 | 4.158 | 26.733 | 1.00 | 30.54 |
| ATOM | 5306 | N | TRP | 684 | 50.902 | 6.332 | 27.282 | 1.00 | 32.57 |
| ATOM | 5308 | CA | TRP | 684 | 49.616 | 6.477 | 26.600 | 1.00 | 32.76 |
| ATOM | 5309 | CB | TRP | 684 | 49.060 | 7.895 | 26.765 | 1.00 | 33.67 |
| ATOM | 5310 | CG | TRP | 684 | 47.855 | 8.210 | 25.891 | 1.00 | 38.22 |
| ATOM | 5311 | CD2 | TRP | 684 | 46.503 | 8.435 | 26.328 | 1.00 | 39.96 |
| ATOM | 5312 | CE2 | TRP | 684 | 45.734 | 8.735 | 25.177 | 1.00 | 39.59 |
| ATOM | 5313 | CE3 | TRP | 684 | 45.869 | 8.416 | 27.578 | 1.00 | 39.26 |
| ATOM | 5314 | CD1 | TRP | 684 | 47.842 | 8.373 | 24.528 | 1.00 | 39.02 |
| ATOM | 5315 | NE1 | TRP | 684 | 46.576 | 8.687 | 24.096 | 1.00 | 38.42 |
| ATOM | 5317 | CZ2 | TRP | 684 | 44.362 | 9.011 | 25.240 | 1.00 | 36.62 |
| ATOM | 5318 | CZ3 | TRP | 684 | 44.502 | 8.691 | 27.641 | 1.00 | 40.70 |
| ATOM | 5319 | CH2 | TRP | 684 | 43.766 | 8.982 | 26.475 | 1.00 | 40.57 |
| ATOM | 5320 | C | TRP | 684 | 49.819 | 6.158 | 25.125 | 1.00 | 31.98 |
| ATOM | 5321 | O | TRP | 684 | 49.066 | 5.367 | 24.557 | 1.00 | 32.43 |
| ATOM | 5322 | N | SER | 685 | 50.859 | 6.748 | 24.529 | 1.00 | 29.63 |
| ATOM | 5324 | CA | SER | 685 | 51.195 | 6.531 | 23.119 | 1.00 | 28.62 |
| ATOM | 5325 | CB | SER | 685 | 52.457 | 7.296 | 22.751 | 1.00 | 24.72 |
| ATOM | 5326 | OG | SER | 685 | 52.323 | 8.664 | 23.072 | 1.00 | 30.04 |
| ATOM | 5328 | C | SER | 685 | 51.414 | 5.055 | 22.825 | 1.00 | 27.91 |
| ATOM | 5329 | O | SER | 685 | 51.022 | 4.555 | 21.767 | 1.00 | 28.60 |
| ATOM | 5330 | N | PHE | 686 | 52.063 | 4.372 | 23.763 | 1.00 | 27.96 |
| ATOM | 5332 | CA | PHE | 686 | 52.333 | 2.947 | 23.662 | 1.00 | 27.03 |
| ATOM | 5333 | CB | PHE | 686 | 53.163 | 2.499 | 24.868 | 1.00 | 25.79 |
| ATOM | 5334 | CG | PHE | 686 | 53.440 | 1.029 | 24.890 | 1.00 | 26.25 |
| ATOM | 5335 | CD1 | PHE | 686 | 54.252 | 0.451 | 23.923 | 1.00 | 27.32 |
| ATOM | 5336 | CD2 | PHE | 686 | 52.839 | 0.208 | 25.841 | 1.00 | 26.22 |
| ATOM | 5337 | CE1 | PHE | 686 | 54.464 | -0.930 | 23.900 | 1.00 | 25.87 |
| ATOM | 5338 | CE2 | PHE | 686 | 53.046 | -1.170 | 25.828 | 1.00 | 24.37 |
| ATOM | 5339 | CZ | PHE | 686 | 53.856 | -1.740 | 24.854 | 1.00 | 26.42 |
| ATOM | 5340 | C | PHE | 686 | 51.003 | 2.160 | 23.596 | 1.00 | 28.82 |
| ATOM | 5341 | O | PHE | 686 | 50.912 | 1.129 | 22.914 | 1.00 | 26.74 |
| ATOM | 5342 | N | GLY | 687 | 49.991 | 2.636 | 24.324 | 1.00 | 29.52 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5344 | CA | GLY | 687 | 48.688 | 1.982 | 24.302 | 1.00 | 31.57 |
| ATOM | 5345 | C | GLY | 687 | 48.095 | 2.036 | 22.896 | 1.00 | 30.73 |
| ATOM | 5346 | O | GLY | 687 | 47.490 | 1.069 | 22.414 | 1.00 | 29.83 |
| ATOM | 5347 | N | VAL | 688 | 48.269 | 3.179 | 22.238 | 1.00 | 29.06 |
| ATOM | 5349 | CA | VAL | 688 | 47.777 | 3.350 | 20.879 | 1.00 | 28.93 |
| ATOM | 5350 | CB | VAL | 688 | 47.800 | 4.831 | 20.424 | 1.00 | 27.24 |
| ATOM | 5351 | CG1 | VAL | 688 | 47.211 | 4.963 | 19.020 | 1.00 | 28.29 |
| ATOM | 5352 | CG2 | VAL | 688 | 46.990 | 5.691 | 21.404 | 1.00 | 26.96 |
| ATOM | 5353 | C | VAL | 688 | 48.612 | 2.475 | 19.951 | 1.00 | 28.49 |
| ATOM | 5354 | O | VAL | 688 | 48.080 | 1.866 | 19.024 | 1.00 | 28.84 |
| ATOM | 5355 | N | LEU | 689 | 49.905 | 2.350 | 20.252 | 1.00 | 27.99 |
| ATOM | 5357 | CA | LEU | 689 | 50.804 | 1.512 | 19.461 | 1.00 | 26.14 |
| ATOM | 5358 | CB | LEU | 689 | 52.268 | 1.688 | 19.911 | 1.00 | 27.31 |
| ATOM | 5359 | CG | LEU | 689 | 53.368 | 1.014 | 19.065 | 1.00 | 26.60 |
| ATOM | 5360 | CD1 | LEU | 689 | 54.688 | 1.767 | 19.175 | 1.00 | 28.19 |
| ATOM | 5361 | CD2 | LEU | 689 | 53.567 | -0.401 | 19.475 | 1.00 | 25.55 |
| ATOM | 5362 | C | LEU | 689 | 50.362 | 0.053 | 19.605 | 1.00 | 26.48 |
| ATOM | 5363 | O | LEU | 689 | 50.377 | -0.686 | 18.626 | 1.00 | 27.06 |
| ATOM | 5364 | N | LEU | 690 | 49.953 | -0.344 | 20.816 | 1.00 | 28.55 |
| ATOM | 5366 | CA | LEU | 690 | 49.465 | -1.708 | 21.085 | 1.00 | 29.16 |
| ATOM | 5367 | CB | LEU | 690 | 49.070 | -1.888 | 22.560 | 1.00 | 31.40 |
| ATOM | 5368 | CG | LEU | 690 | 50.114 | -2.085 | 23.667 | 1.00 | 31.49 |
| ATOM | 5369 | CD1 | LEU | 690 | 49.427 | -2.028 | 25.026 | 1.00 | 34.09 |
| ATOM | 5370 | CD2 | LEU | 690 | 50.821 | -3.410 | 23.491 | 1.00 | 30.84 |
| ATOM | 5371 | C | LEU | 690 | 48.240 | -1.958 | 20.220 | 1.00 | 26.51 |
| ATOM | 5372 | O | LEU | 690 | 48.088 | -3.023 | 19.631 | 1.00 | 25.15 |
| ATOM | 5373 | N | TRP | 691 | 47.376 | -0.954 | 20.139 | 1.00 | 28.51 |
| ATOM | 5375 | CA | TRP | 691 | 46.169 | -1.049 | 19.319 | 1.00 | 29.56 |
| ATOM | 5376 | CB | TRP | 691 | 45.332 | 0.227 | 19.465 | 1.00 | 28.91 |
| ATOM | 5377 | CG | TRP | 691 | 43.992 | 0.169 | 18.759 | 1.00 | 30.95 |
| ATOM | 5378 | CD2 | TRP | 691 | 43.718 | 0.556 | 17.406 | 1.00 | 29.87 |
| ATOM | 5379 | CE2 | TRP | 691 | 42.337 | 0.367 | 17.189 | 1.00 | 31.97 |
| ATOM | 5380 | CE3 | TRP | 691 | 44.505 | 1.049 | 16.358 | 1.00 | 27.72 |
| ATOM | 5381 | CD1 | TRP | 691 | 42.796 | -0.231 | 19.292 | 1.00 | 30.68 |
| ATOM | 5382 | NE1 | TRP | 691 | 41.797 | -0.111 | 18.355 | 1.00 | 33.68 |
| ATOM | 5384 | CZ2 | TRP | 691 | 41.729 | 0.652 | 15.967 | 1.00 | 29.42 |
| ATOM | 5385 | CZ3 | TRP | 691 | 43.906 | 1.327 | 15.154 | 1.00 | 27.13 |
| ATOM | 5386 | CH2 | TRP | 691 | 42.523 | 1.129 | 14.965 | 1.00 | 29.18 |
| ATOM | 5387 | C | TRP | 691 | 46.564 | -1.289 | 17.856 | 1.00 | 28.78 |
| ATOM | 5388 | O | TRP | 691 | 45.996 | -2.156 | 17.194 | 1.00 | 27.64 |
| ATOM | 5389 | N | GLU | 692 | 47.564 | -0.543 | 17.380 | 1.00 | 29.83 |
| ATOM | 5391 | CA | GLU | 692 | 48.078 | -0.669 | 16.018 | 1.00 | 28.08 |
| ATOM | 5392 | CB | GLU | 692 | 49.267 | 0.262 | 15.790 | 1.00 | 26.40 |
| ATOM | 5393 | CG | GLU | 692 | 48.945 | 1.735 | 15.680 | 1.00 | 26.45 |
| ATOM | 5394 | CD | GLU | 692 | 50.183 | 2.561 | 15.369 | 1.00 | 29.47 |
| ATOM | 5395 | OE1 | GLU | 692 | 50.938 | 2.886 | 16.320 | 1.00 | 29.66 |
| ATOM | 5396 | OE2 | GLU | 692 | 50.413 | 2.875 | 14.182 | 1.00 | 29.44 |
| ATOM | 5397 | C | GLU | 692 | 48.563 | -2.082 | 15.761 | 1.00 | 30.07 |
| ATOM | 5398 | O | GLU | 692 | 48.385 | -2.612 | 14.665 | 1.00 | 30.18 |
| ATOM | 5399 | N | ILE | 693 | 49.244 | -2.663 | 16.746 | 1.00 | 29.87 |
| ATOM | 5401 | CA | ILE | 693 | 49.754 | -4.024 | 16.608 | 1.00 | 29.51 |
| ATOM | 5402 | CB | ILE | 693 | 50.632 | -4.443 | 17.828 | 1.00 | 28.18 |
| ATOM | 5403 | CG2 | ILE | 693 | 51.037 | -5.907 | 17.706 | 1.00 | 27.45 |
| ATOM | 5404 | CG1 | ILE | 693 | 51.907 | -3.594 | 17.890 | 1.00 | 26.99 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5405 | CD1 | ILE | 693 | 52.663 | -3.747 | 19.194 | 1.00 | 25.37 |
| ATOM | 5406 | C | ILE | 693 | 48.603 | -5.023 | 16.452 | 1.00 | 29.21 |
| ATOM | 5407 | O | ILE | 693 | 48.568 | -5.807 | 15.512 | 1.00 | 27.89 |
| ATOM | 5408 | N | PHE | 694 | 47.623 | -4.942 | 17.336 | 1.00 | 31.33 |
| ATOM | 5410 | CA | PHE | 694 | 46.523 | -5.888 | 17.279 | 1.00 | 34.41 |
| ATOM | 5411 | CB | PHE | 694 | 45.958 | -6.114 | 18.687 | 1.00 | 35.37 |
| ATOM | 5412 | CG | PHE | 694 | 46.978 | -6.717 | 19.621 | 1.00 | 35.60 |
| ATOM | 5413 | CD1 | PHE | 694 | 47.606 | -5.942 | 20.586 | 1.00 | 37.23 |
| ATOM | 5414 | CD2 | PHE | 694 | 47.424 | -8.024 | 19.426 | 1.00 | 35.59 |
| ATOM | 5415 | CE1 | PHE | 694 | 48.669 | -6.460 | 21.333 | 1.00 | 36.39 |
| ATOM | 5416 | CE2 | PHE | 694 | 48.484 | -8.546 | 20.170 | 1.00 | 35.34 |
| ATOM | 5417 | CZ | PHE | 694 | 49.110 | -7.762 | 21.118 | 1.00 | 35.71 |
| ATOM | 5418 | C | PHE | 694 | 45.481 | -5.715 | 16.176 | 1.00 | 34.41 |
| ATOM | 5419 | O | PHE | 694 | 44.623 | -6.579 | 15.982 | 1.00 | 34.48 |
| ATOM | 5420 | N | THR | 695 | 45.617 | -4.637 | 15.404 | 1.00 | 33.03 |
| ATOM | 5422 | CA | THR | 695 | 44.742 | -4.379 | 14.263 | 1.00 | 31.81 |
| ATOM | 5423 | CB | THR | 695 | 44.113 | -2.957 | 14.278 | 1.00 | 29.75 |
| ATOM | 5424 | OG1 | THR | 695 | 45.142 | -1.961 | 14.218 | 1.00 | 30.72 |
| ATOM | 5426 | CG2 | THR | 695 | 43.254 | -2.759 | 15.524 | 1.00 | 29.40 |
| ATOM | 5427 | C | THR | 695 | 45.596 | -4.533 | 13.011 | 1.00 | 31.44 |
| ATOM | 5428 | O | THR | 695 | 45.153 | -4.241 | 11.906 | 1.00 | 33.00 |
| ATOM | 5429 | N | LEU | 696 | 46.832 | -4.987 | 13.209 | 1.00 | 31.24 |
| ATOM | 5431 | CA | LEU | 696 | 47.799 | -5.199 | 12.134 | 1.00 | 31.36 |
| ATOM | 5432 | CB | LEU | 696 | 47.421 | -6.418 | 11.291 | 1.00 | 33.53 |
| ATOM | 5433 | CG | LEU | 696 | 47.270 | -7.741 | 12.042 | 1.00 | 33.00 |
| ATOM | 5434 | CD1 | LEU | 696 | 47.010 | -8.838 | 11.052 | 1.00 | 35.50 |
| ATOM | 5435 | CD2 | LEU | 696 | 48.515 | -8.061 | 12.830 | 1.00 | 36.09 |
| ATOM | 5436 | C | LEU | 696 | 48.066 | -3.976 | 11.249 | 1.00 | 30.84 |
| ATOM | 5437 | O | LEU | 696 | 48.135 | -4.067 | 10.024 | 1.00 | 28.23 |
| ATOM | 5438 | N | GLY | 697 | 48.302 | -2.839 | 11.890 | 1.00 | 31.54 |
| ATOM | 5440 | CA | GLY | 697 | 48.591 | -1.632 | 11.141 | 1.00 | 33.87 |
| ATOM | 5441 | C | GLY | 697 | 47.375 | -0.765 | 10.924 | 1.00 | 32.77 |
| ATOM | 5442 | O | GLY | 697 | 47.322 | 0.042 | 9.994 | 1.00 | 33.90 |
| ATOM | 5443 | N | GLY | 698 | 46.392 | -0.921 | 11.797 | 1.00 | 33.29 |
| ATOM | 5445 | CA | GLY | 698 | 45.187 | -0.122 | 11.681 | 1.00 | 32.66 |
| ATOM | 5446 | C | GLY | 698 | 45.408 | 1.368 | 11.877 | 1.00 | 30.57 |
| ATOM | 5447 | O | GLY | 698 | 46.336 | 1.803 | 12.553 | 1.00 | 27.36 |
| ATOM | 5448 | N | SER | 699 | 44.517 | 2.148 | 11.285 | 1.00 | 30.92 |
| ATOM | 5450 | CA | SER | 699 | 44.552 | 3.595 | 11.376 | 1.00 | 32.19 |
| ATOM | 5451 | CB | SER | 699 | 44.062 | 4.202 | 10.058 | 1.00 | 34.24 |
| ATOM | 5452 | OG | SER | 699 | 44.019 | 5.616 | 10.123 | 1.00 | 38.67 |
| ATOM | 5454 | C | SER | 699 | 43.644 | 4.014 | 12.538 | 1.00 | 31.81 |
| ATOM | 5455 | O | SER | 699 | 42.431 | 3.759 | 12.525 | 1.00 | 31.39 |
| ATOM | 5456 | N | PRO | 700 | 44.228 | 4.597 | 13.594 | 1.00 | 31.82 |
| ATOM | 5457 | CD | PRO | 700 | 45.645 | 4.842 | 13.919 | 1.00 | 28.82 |
| ATOM | 5458 | CA | PRO | 700 | 43.353 | 4.992 | 14.697 | 1.00 | 31.31 |
| ATOM | 5459 | CB | PRO | 700 | 44.345 | 5.341 | 15.809 | 1.00 | 31.31 |
| ATOM | 5460 | CG | PRO | 700 | 45.552 | 5.800 | 15.061 | 1.00 | 30.41 |
| ATOM | 5461 | C | PRO | 700 | 42.484 | 6.170 | 14.295 | 1.00 | 31.19 |
| ATOM | 5462 | O | PRO | 700 | 42.899 | 7.021 | 13.510 | 1.00 | 29.93 |
| ATOM | 5463 | N | TYR | 701 | 41.235 | 6.144 | 14.736 | 1.00 | 32.69 |
| ATOM | 5465 | CA | TYR | 701 | 40.291 | 7.223 | 14.445 | 1.00 | 32.54 |
| ATOM | 5466 | CB | TYR | 701 | 40.650 | 8.416 | 15.323 | 1.00 | 34.47 |
| ATOM | 5467 | CG | TYR | 701 | 40.512 | 8.141 | 16.794 | 1.00 | 39.16 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5468 | CD1 | TYR | 701 | 41.542 | 8.433 | 17.683 | 1.00 | 44.31 |
| ATOM | 5469 | CE1 | TYR | 701 | 41.372 | 8.241 | 19.060 | 1.00 | 46.65 |
| ATOM | 5470 | CD2 | TYR | 701 | 39.321 | 7.642 | 17.307 | 1.00 | 41.21 |
| ATOM | 5471 | CE2 | TYR | 701 | 39.147 | 7.447 | 18.657 | 1.00 | 45.05 |
| ATOM | 5472 | CZ | TYR | 701 | 40.164 | 7.750 | 19.535 | 1.00 | 47.24 |
| ATOM | 5473 | OH | TYR | 701 | 39.949 | 7.590 | 20.886 | 1.00 | 52.18 |
| ATOM | 5475 | C | TYR | 701 | 40.215 | 7.655 | 12.972 | 1.00 | 30.56 |
| ATOM | 5476 | O | TYR | 701 | 40.379 | 8.836 | 12.647 | 1.00 | 29.73 |
| ATOM | 5477 | N | PRO | 702 | 39.928 | 6.712 | 12.058 | 1.00 | 30.38 |
| ATOM | 5478 | CD | PRO | 702 | 39.659 | 5.278 | 12.261 | 1.00 | 30.22 |
| ATOM | 5479 | CA | PRO | 702 | 39.847 | 7.071 | 10.642 | 1.00 | 28.87 |
| ATOM | 5480 | CB | PRO | 702 | 39.693 | 5.722 | 9.948 | 1.00 | 29.63 |
| ATOM | 5481 | CG | PRO | 702 | 39.007 | 4.889 | 10.959 | 1.00 | 30.99 |
| ATOM | 5482 | C | PRO | 702 | 38.722 | 8.048 | 10.283 | 1.00 | 30.88 |
| ATOM | 5483 | O | PRO | 702 | 37.557 | 7.843 | 10.636 | 1.00 | 33.98 |
| ATOM | 5484 | N | GLY | 703 | 39.100 | 9.116 | 9.584 | 1.00 | 29.03 |
| ATOM | 5486 | CA | GLY | 703 | 38.154 | 10.134 | 9.169 | 1.00 | 28.98 |
| ATOM | 5487 | C | GLY | 703 | 37.893 | 11.169 | 10.244 | 1.00 | 29.69 |
| ATOM | 5488 | O | GLY | 703 | 37.074 | 12.068 | 10.048 | 1.00 | 31.71 |
| ATOM | 5489 | N | VAL | 704 | 38.579 | 11.040 | 11.378 | 1.00 | 30.74 |
| ATOM | 5491 | CA | VAL | 704 | 38.416 | 11.951 | 12.509 | 1.00 | 32.06 |
| ATOM | 5492 | CB | VAL | 704 | 38.582 | 11.208 | 13.860 | 1.00 | 31.70 |
| ATOM | 5493 | CG1 | VAL | 704 | 38.522 | 12.197 | 15.044 | 1.00 | 30.29 |
| ATOM | 5494 | CG2 | VAL | 704 | 37.506 | 10.144 | 14.005 | 1.00 | 31.56 |
| ATOM | 5495 | C | VAL | 704 | 39.430 | 13.087 | 12.449 | 1.00 | 33.72 |
| ATOM | 5496 | O | VAL | 704 | 40.634 | 12.867 | 12.548 | 1.00 | 35.31 |
| ATOM | 5497 | N | PRO | 705 | 38.957 | 14.309 | 12.200 | 1.00 | 34.23 |
| ATOM | 5498 | CD | PRO | 705 | 37.594 | 14.692 | 11.787 | 1.00 | 33.20 |
| ATOM | 5499 | CA | PRO | 705 | 39.875 | 15.443 | 12.135 | 1.00 | 33.73 |
| ATOM | 5500 | CB | PRO | 705 | 39.053 | 16.495 | 11.394 | 1.00 | 34.93 |
| ATOM | 5501 | CG | PRO | 705 | 37.647 | 16.187 | 11.831 | 1.00 | 36.93 |
| ATOM | 5502 | C | PRO | 705 | 40.280 | 15.879 | 13.543 | 1.00 | 33.25 |
| ATOM | 5503 | O | PRO | 705 | 39.651 | 15.490 | 14.532 | 1.00 | 31.71 |
| ATOM | 5504 | N | VAL | 706 | 41.322 | 16.697 | 13.623 | 1.00 | 34.46 |
| ATOM | 5506 | CA | VAL | 706 | 41.852 | 17.176 | 14.900 | 1.00 | 36.99 |
| ATOM | 5507 | CB | VAL | 706 | 42.923 | 18.261 | 14.687 | 1.00 | 39.01 |
| ATOM | 5508 | CG1 | VAL | 706 | 43.577 | 18.618 | 16.017 | 1.00 | 40.33 |
| ATOM | 5509 | CG2 | VAL | 706 | 43.961 | 17.786 | 13.673 | 1.00 | 38.61 |
| ATOM | 5510 | C | VAL | 706 | 40.826 | 17.716 | 15.895 | 1.00 | 35.65 |
| ATOM | 5511 | O | VAL | 706 | 40.823 | 17.319 | 17.065 | 1.00 | 33.55 |
| ATOM | 5512 | N | GLU | 707 | 39.955 | 18.605 | 15.426 | 1.00 | 36.74 |
| ATOM | 5514 | CA | GLU | 707 | 38.941 | 19.220 | 16.278 | 1.00 | 37.20 |
| ATOM | 5515 | CB | GLU | 707 | 38.129 | 20.242 | 15.482 | 1.00 | 38.98 |
| ATOM | 5516 | C | GLU | 707 | 38.014 | 18.188 | 16.900 | 1.00 | 38.46 |
| ATOM | 5517 | O | GLU | 707 | 37.634 | 18.295 | 18.074 | 1.00 | 39.04 |
| ATOM | 5518 | N | GLU | 708 | 37.681 | 17.170 | 16.115 | 1.00 | 37.81 |
| ATOM | 5520 | CA | GLU | 708 | 36.802 | 16.105 | 16.571 | 1.00 | 37.70 |
| ATOM | 5521 | CB | GLU | 708 | 36.316 | 15.289 | 15.378 | 1.00 | 40.73 |
| ATOM | 5522 | CG | GLU | 708 | 35.459 | 16.091 | 14.413 | 1.00 | 43.44 |
| ATOM | 5523 | CD | GLU | 708 | 34.235 | 16.677 | 15.084 | 1.00 | 51.52 |
| ATOM | 5524 | OE1 | GLU | 708 | 33.629 | 16.007 | 15.961 | 1.00 | 50.14 |
| ATOM | 5525 | OE2 | GLU | 708 | 33.882 | 17.824 | 14.732 | 1.00 | 59.46 |
| ATOM | 5526 | C | GLU | 708 | 37.506 | 15.223 | 17.588 | 1.00 | 36.53 |
| ATOM | 5527 | O | GLU | 708 | 36.897 | 14.782 | 18.567 | 1.00 | 36.80 |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5528 | N | LEU | 709 | 38.799 | 14.993 | 17.376 | 1.00 | 35.69 |
| ATOM | 5530 | CA | LEU | 709 | 39.584 | 14.179 | 18.301 | 1.00 | 35.48 |
| ATOM | 5531 | CB | LEU | 709 | 41.039 | 14.044 | 17.830 | 1.00 | 34.84 |
| ATOM | 5532 | CG | LEU | 709 | 41.921 | 13.250 | 18.802 | 1.00 | 32.41 |
| ATOM | 5533 | CD1 | LEU | 709 | 41.608 | 11.787 | 18.674 | 1.00 | 30.10 |
| ATOM | 5534 | CD2 | LEU | 709 | 43.378 | 13.514 | 18.560 | 1.00 | 29.93 |
| ATOM | 5535 | C | LEU | 709 | 39.568 | 14.842 | 19.673 | 1.00 | 35.58 |
| ATOM | 5536 | O | LEU | 709 | 39.377 | 14.177 | 20.694 | 1.00 | 35.43 |
| ATOM | 5537 | N | PHE | 710 | 39.792 | 16.150 | 19.686 | 1.00 | 36.79 |
| ATOM | 5539 | CA | PHE | 710 | 39.800 | 16.918 | 20.927 | 1.00 | 40.58 |
| ATOM | 5540 | CB | PHE | 710 | 39.944 | 18.413 | 20.637 | 1.00 | 42.55 |
| ATOM | 5541 | CG | PHE | 710 | 41.308 | 18.808 | 20.162 | 1.00 | 46.38 |
| ATOM | 5542 | CD1 | PHE | 710 | 42.392 | 17.942 | 20.313 | 1.00 | 47.29 |
| ATOM | 5543 | CD2 | PHE | 710 | 41.515 | 20.050 | 19.580 | 1.00 | 47.93 |
| ATOM | 5544 | CE1 | PHE | 710 | 43.659 | 18.312 | 19.892 | 1.00 | 51.21 |
| ATOM | 5545 | CE2 | PHE | 710 | 42.781 | 20.435 | 19.155 | 1.00 | 50.89 |
| ATOM | 5546 | CZ | PHE | 710 | 43.859 | 19.562 | 19.312 | 1.00 | 53.31 |
| ATOM | 5547 | C | PHE | 710 | 38.517 | 16.676 | 21.694 | 1.00 | 40.14 |
| ATOM | 5548 | O | PHE | 710 | 38.543 | 16.446 | 22.898 | 1.00 | 39.86 |
| ATOM | 5549 | N | LYS | 711 | 37.399 | 16.705 | 20.977 | 1.00 | 41.02 |
| ATOM | 5551 | CA | LYS | 711 | 36.101 | 16.479 | 21.584 | 1.00 | 38.66 |
| ATOM | 5552 | CB | LYS | 711 | 34.985 | 16.803 | 20.580 | 1.00 | 40.75 |
| ATOM | 5553 | CG | LYS | 711 | 33.601 | 16.727 | 21.181 | 1.00 | 46.99 |
| ATOM | 5554 | CD | LYS | 711 | 32.522 | 17.174 | 20.218 | 1.00 | 50.71 |
| ATOM | 5555 | CE | LYS | 711 | 31.163 | 16.733 | 20.739 | 1.00 | 52.53 |
| ATOM | 5556 | NZ | LYS | 711 | 30.041 | 17.194 | 19.884 | 1.00 | 57.76 |
| ATOM | 5560 | C | LYS | 711 | 35.990 | 15.046 | 22.120 | 1.00 | 38.06 |
| ATOM | 5561 | O | LYS | 711 | 35.535 | 14.831 | 23.250 | 1.00 | 36.29 |
| ATOM | 5562 | N | LEU | 712 | 36.431 | 14.066 | 21.330 | 1.00 | 38.10 |
| ATOM | 5564 | CA | LEU | 712 | 36.392 | 12.662 | 21.764 | 1.00 | 38.69 |
| ATOM | 5565 | CB | LEU | 712 | 36.914 | 11.714 | 20.672 | 1.00 | 37.19 |
| ATOM | 5566 | CG | LEU | 712 | 36.070 | 11.436 | 19.424 | 1.00 | 34.73 |
| ATOM | 5567 | CD1 | LEU | 712 | 36.814 | 10.453 | 18.524 | 1.00 | 35.54 |
| ATOM | 5568 | CD2 | LEU | 712 | 34.709 | 10.872 | 19.818 | 1.00 | 30.90 |
| ATOM | 5569 | C | LEU | 712 | 37.230 | 12.472 | 23.021 | 1.00 | 39.62 |
| ATOM | 5570 | O | LEU | 712 | 36.843 | 11.745 | 23.940 | 1.00 | 39.44 |
| ATOM | 5571 | N | LEU | 713 | 38.398 | 13.101 | 23.044 | 1.00 | 40.10 |
| ATOM | 5573 | CA | LEU | 713 | 39.279 | 12.999 | 24.199 | 1.00 | 42.81 |
| ATOM | 5574 | CB | LEU | 713 | 40.606 | 13.716 | 23.924 | 1.00 | 41.70 |
| ATOM | 5575 | CG | LEU | 713 | 41.495 | 13.040 | 22.868 | 1.00 | 41.86 |
| ATOM | 5576 | CD1 | LEU | 713 | 42.742 | 13.862 | 22.607 | 1.00 | 37.19 |
| ATOM | 5577 | CD2 | LEU | 713 | 41.873 | 11.647 | 23.340 | 1.00 | 41.17 |
| ATOM | 5578 | C | LEU | 713 | 38.577 | 13.566 | 25.437 | 1.00 | 43.18 |
| ATOM | 5579 | O | LEU | 713 | 38.479 | 12.889 | 26.457 | 1.00 | 44.79 |
| ATOM | 5580 | N | LYS | 714 | 38.004 | 14.760 | 25.312 | 1.00 | 42.75 |
| ATOM | 5582 | CA | LYS | 714 | 37.301 | 15.389 | 26.425 | 1.00 | 43.70 |
| ATOM | 5583 | CB | LYS | 714 | 36.842 | 16.796 | 26.043 | 1.00 | 44.69 |
| ATOM | 5584 | CG | LYS | 714 | 38.001 | 17.746 | 25.836 | 1.00 | 47.92 |
| ATOM | 5585 | CD | LYS | 714 | 37.543 | 19.171 | 25.583 | 1.00 | 55.01 |
| ATOM | 5586 | CE | LYS | 714 | 38.733 | 20.077 | 25.238 | 1.00 | 59.44 |
| ATOM | 5587 | NZ | LYS | 714 | 39.773 | 20.132 | 26.320 | 1.00 | 60.10 |
| ATOM | 5591 | C | LYS | 714 | 36.127 | 14.557 | 26.940 | 1.00 | 43.94 |
| ATOM | 5592 | O | LYS | 714 | 35.843 | 14.551 | 28.140 | 1.00 | 44.20 |
| ATOM | 5593 | N | GLU | 715 | 35.477 | 13.819 | 26.046 | 1.00 | 43.29 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5595 | CA | GLU | 715 | 34.350 | 12.979 | 26.435 | 1.00 | 42.29 |
| ATOM | 5596 | CB | GLU | 715 | 33.464 | 12.682 | 25.225 | 1.00 | 44.91 |
| ATOM | 5597 | CG | GLU | 715 | 32.913 | 13.916 | 24.522 | 1.00 | 51.62 |
| ATOM | 5598 | CD | GLU | 715 | 32.020 | 13.566 | 23.332 | 1.00 | 55.01 |
| ATOM | 5599 | OE1 | GLU | 715 | 32.343 | 12.605 | 22.596 | 1.00 | 58.09 |
| ATOM | 5600 | OE2 | GLU | 715 | 30.992 | 14.251 | 23.136 | 1.00 | 55.83 |
| ATOM | 5601 | C | GLU | 715 | 34.806 | 11.665 | 27.064 | 1.00 | 41.07 |
| ATOM | 5602 | O | GLU | 715 | 33.982 | 10.825 | 27.421 | 1.00 | 38.01 |
| ATOM | 5603 | N | GLY | 716 | 36.118 | 11.476 | 27.182 | 1.00 | 41.11 |
| ATOM | 5605 | CA | GLY | 716 | 36.642 | 10.252 | 27.770 | 1.00 | 39.69 |
| ATOM | 5606 | C | GLY | 716 | 36.510 | 9.054 | 26.847 | 1.00 | 39.64 |
| ATOM | 5607 | O | GLY | 716 | 36.562 | 7.904 | 27.290 | 1.00 | 36.71 |
| ATOM | 5608 | N | HIS | 717 | 36.359 | 9.335 | 25.554 | 1.00 | 41.95 |
| ATOM | 5610 | CA | HIS | 717 | 36.215 | 8.300 | 24.541 | 1.00 | 43.32 |
| ATOM | 5611 | CB | HIS | 717 | 35.859 | 8.918 | 23.183 | 1.00 | 43.38 |
| ATOM | 5612 | CG | HIS | 717 | 35.813 | 7.926 | 22.060 | 1.00 | 44.79 |
| ATOM | 5613 | CD2 | HIS | 717 | 34.802 | 7.152 | 21.596 | 1.00 | 44.64 |
| ATOM | 5614 | ND1 | HIS | 717 | 36.912 | 7.625 | 21.285 | 1.00 | 46.21 |
| ATOM | 5616 | CE1 | HIS | 717 | 36.584 | 6.708 | 20.392 | 1.00 | 46.21 |
| ATOM | 5617 | NE2 | HIS | 717 | 35.307 | 6.404 | 20.561 | 1.00 | 45.55 |
| ATOM | 5619 | C | HIS | 717 | 37.485 | 7.481 | 24.403 | 1.00 | 43.90 |
| ATOM | 5620 | O | HIS | 717 | 38.581 | 8.031 | 24.327 | 1.00 | 45.45 |
| ATOM | 5621 | N | ARG | 718 | 37.304 | 6.169 | 24.289 | 1.00 | 43.44 |
| ATOM | 5623 | CA | ARG | 718 | 38.387 | 5.207 | 24.139 | 1.00 | 42.68 |
| ATOM | 5624 | CB | ARG | 718 | 38.500 | 4.361 | 25.412 | 1.00 | 41.00 |
| ATOM | 5625 | CG | ARG | 718 | 38.844 | 5.165 | 26.658 | 1.00 | 40.09 |
| ATOM | 5626 | CD | ARG | 718 | 40.214 | 5.825 | 26.495 | 1.00 | 41.06 |
| ATOM | 5627 | NE | ARG | 718 | 40.658 | 6.549 | 27.685 | 1.00 | 39.51 |
| ATOM | 5629 | CZ | ARG | 718 | 40.521 | 7.861 | 27.862 | 1.00 | 39.90 |
| ATOM | 5630 | NH1 | ARG | 718 | 39.940 | 8.608 | 26.931 | 1.00 | 36.48 |
| ATOM | 5633 | NH2 | ARG | 718 | 41.024 | 8.443 | 28.946 | 1.00 | 42.06 |
| ATOM | 5636 | C | ARG | 718 | 38.080 | 4.308 | 22.927 | 1.00 | 43.91 |
| ATOM | 5637 | O | ARG | 718 | 36.911 | 4.007 | 22.650 | 1.00 | 44.40 |
| ATOM | 5638 | N | MET | 719 | 39.113 | 3.933 | 22.174 | 1.00 | 42.56 |
| ATOM | 5640 | CA | MET | 719 | 38.928 | 3.079 | 21.004 | 1.00 | 42.82 |
| ATOM | 5641 | CB | MET | 719 | 40.219 | 2.964 | 20.181 | 1.00 | 42.59 |
| ATOM | 5642 | CG | MET | 719 | 40.595 | 4.221 | 19.413 | 1.00 | 41.15 |
| ATOM | 5643 | SD | MET | 719 | 42.093 | 4.079 | 18.400 | 1.00 | 44.11 |
| ATOM | 5644 | CE | MET | 719 | 43.323 | 3.949 | 19.613 | 1.00 | 41.33 |
| ATOM | 5645 | C | MET | 719 | 38.460 | 1.694 | 21.432 | 1.00 | 44.74 |
| ATOM | 5646 | O | MET | 719 | 38.822 | 1.216 | 22.516 | 1.00 | 41.56 |
| ATOM | 5647 | N | ASP | 720 | 37.635 | 1.075 | 20.582 | 1.00 | 45.50 |
| ATOM | 5649 | CA | ASP | 720 | 37.090 | -0.265 | 20.824 | 1.00 | 45.51 |
| ATOM | 5650 | CB | ASP | 720 | 36.077 | -0.660 | 19.733 | 1.00 | 48.60 |
| ATOM | 5651 | CG | ASP | 720 | 34.811 | 0.181 | 19.749 | 1.00 | 53.03 |
| ATOM | 5652 | OD1 | ASP | 720 | 34.678 | 1.082 | 20.612 | 1.00 | 59.61 |
| ATOM | 5653 | OD2 | ASP | 720 | 33.943 | -0.067 | 18.880 | 1.00 | 50.58 |
| ATOM | 5654 | C | ASP | 720 | 38.177 | -1.329 | 20.823 | 1.00 | 43.64 |
| ATOM | 5655 | O | ASP | 720 | 39.235 | -1.172 | 20.199 | 1.00 | 43.66 |
| ATOM | 5656 | N | LYS | 721 | 37.876 | -2.436 | 21.487 | 1.00 | 42.90 |
| ATOM | 5658 | CA | LYS | 721 | 38.784 | -3.565 | 21.555 | 1.00 | 42.96 |
| ATOM | 5659 | CB | LYS | 721 | 38.278 | -4.565 | 22.587 | 1.00 | 42.51 |
| ATOM | 5660 | CG | LYS | 721 | 39.000 | -5.888 | 22.570 | 1.00 | 47.68 |
| ATOM | 5661 | CD | LYS | 721 | 38.445 | -6.805 | 23.628 | 1.00 | 51.61 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5662 | CE | LYS | 721 | 38.450 | -8.246 | 23.163 | 1.00 | 54.96 |
| ATOM | 5663 | NZ | LYS | 721 | 38.165 | -9.190 | 24.282 | 1.00 | 59.67 |
| ATOM | 5667 | C | LYS | 721 | 38.825 | -4.215 | 20.182 | 1.00 | 43.05 |
| ATOM | 5668 | O | LYS | 721 | 37.779 | -4.577 | 19.625 | 1.00 | 46.08 |
| ATOM | 5669 | N | PRO | 722 | 40.025 | -4.348 | 19.601 | 1.00 | 43.22 |
| ATOM | 5670 | CD | PRO | 722 | 41.337 | -3.872 | 20.067 | 1.00 | 43.52 |
| ATOM | 5671 | CA | PRO | 722 | 40.139 | -4.968 | 18.275 | 1.00 | 41.04 |
| ATOM | 5672 | CB | PRO | 722 | 41.631 | -4.856 | 17.965 | 1.00 | 40.87 |
| ATOM | 5673 | CG | PRO | 722 | 42.074 | -3.682 | 18.764 | 1.00 | 42.22 |
| ATOM | 5674 | C | PRO | 722 | 39.726 | -6.427 | 18.346 | 1.00 | 39.64 |
| ATOM | 5675 | O | PRO | 722 | 39.730 | -7.023 | 19.425 | 1.00 | 37.12 |
| ATOM | 5676 | N | SER | 723 | 39.311 | -6.982 | 17.212 | 1.00 | 40.36 |
| ATOM | 5678 | CA | SER | 723 | 38.947 | -8.389 | 17.158 | 1.00 | 41.41 |
| ATOM | 5679 | CB | SER | 723 | 38.205 | -8.707 | 15.865 | 1.00 | 38.26 |
| ATOM | 5680 | OG | SER | 723 | 39.049 | -8.520 | 14.749 | 1.00 | 43.87 |
| ATOM | 5682 | C | SER | 723 | 40.294 | -9.102 | 17.191 | 1.00 | 41.54 |
| ATOM | 5683 | O | SER | 723 | 41.284 | -8.575 | 16.703 | 1.00 | 40.90 |
| ATOM | 5684 | N | ASN | 724 | 40.338 | -10.300 | 17.750 | 1.00 | 44.89 |
| ATOM | 5686 | CA | ASN | 724 | 41.598 | -11.019 | 17.853 | 1.00 | 48.14 |
| ATOM | 5687 | CB | ASN | 724 | 42.256 | -11.202 | 16.476 | 1.00 | 52.43 |
| ATOM | 5688 | CG | ASN | 724 | 41.682 | -12.374 | 15.715 | 1.00 | 57.29 |
| ATOM | 5689 | OD1 | ASN | 724 | 41.637 | -13.492 | 16.225 | 1.00 | 61.96 |
| ATOM | 5690 | ND2 | ASN | 724 | 41.218 | -12.125 | 14.500 | 1.00 | 60.91 |
| ATOM | 5693 | C | ASN | 724 | 42.509 | -10.255 | 18.811 | 1.00 | 48.17 |
| ATOM | 5694 | O | ASN | 724 | 43.648 | -9.918 | 18.495 | 1.00 | 49.88 |
| ATOM | 5695 | N | CYS | 725 | 41.960 | -9.935 | 19.973 | 1.00 | 47.12 |
| ATOM | 5697 | CA | CYS | 725 | 42.686 | -9.238 | 21.010 | 1.00 | 46.17 |
| ATOM | 5698 | CB | CYS | 725 | 42.569 | -7.717 | 20.862 | 1.00 | 44.83 |
| ATOM | 5699 | SG | CYS | 725 | 43.459 | -6.813 | 22.159 | 1.00 | 42.51 |
| ATOM | 5700 | C | CYS | 725 | 42.017 | -9.697 | 22.294 | 1.00 | 45.78 |
| ATOM | 5701 | O | CYS | 725 | 40.803 | -9.642 | 22.423 | 1.00 | 44.83 |
| ATOM | 5702 | N | THR | 726 | 42.810 | -10.224 | 23.212 | 1.00 | 45.63 |
| ATOM | 5704 | CA | THR | 726 | 42.289 | -10.711 | 24.482 | 1.00 | 45.47 |
| ATOM | 5705 | CB | THR | 726 | 43.351 | -11.545 | 25.217 | 1.00 | 45.93 |
| ATOM | 5706 | OG1 | THR | 726 | 44.307 | -10.651 | 25.786 | 1.00 | 45.04 |
| ATOM | 5708 | CG2 | THR | 726 | 44.061 | -12.495 | 24.233 | 1.00 | 42.99 |
| ATOM | 5709 | C | THR | 726 | 41.858 | -9.545 | 25.359 | 1.00 | 45.73 |
| ATOM | 5710 | O | THR | 726 | 42.368 | -8.445 | 25.216 | 1.00 | 46.91 |
| ATOM | 5711 | N | ASN | 727 | 40.914 | -9.789 | 26.257 | 1.00 | 45.93 |
| ATOM | 5713 | CA | ASN | 727 | 40.448 | -8.736 | 27.141 | 1.00 | 47.85 |
| ATOM | 5714 | CB | ASN | 727 | 39.300 | -9.237 | 28.022 | 1.00 | 54.88 |
| ATOM | 5715 | CG | ASN | 727 | 39.629 | -10.544 | 28.731 | 1.00 | 65.11 |
| ATOM | 5716 | OD1 | ASN | 727 | 40.737 | -10.734 | 29.229 | 1.00 | 70.58 |
| ATOM | 5717 | ND2 | ASN | 727 | 38.681 | -11.472 | 28.735 | 1.00 | 69.68 |
| ATOM | 5720 | C | ASN | 727 | 41.591 | -8.212 | 27.999 | 1.00 | 44.18 |
| ATOM | 5721 | O | ASN | 727 | 41.594 | -7.047 | 28.390 | 1.00 | 41.35 |
| ATOM | 5722 | N | GLU | 728 | 42.572 | -9.073 | 28.260 | 1.00 | 42.82 |
| ATOM | 5724 | CA | GLU | 728 | 43.725 | -8.713 | 29.071 | 1.00 | 42.37 |
| ATOM | 5725 | CB | GLU | 728 | 44.573 | -9.952 | 29.379 | 1.00 | 43.09 |
| ATOM | 5726 | CG | GLU | 728 | 45.806 | -9.654 | 30.245 | 1.00 | 48.30 |
| ATOM | 5727 | CD | GLU | 728 | 46.643 | -10.889 | 30.568 | 1.00 | 50.11 |
| ATOM | 5728 | OE1 | GLU | 728 | 46.867 | -11.732 | 29.668 | 1.00 | 47.98 |
| ATOM | 5729 | OE2 | GLU | 728 | 47.085 | -11.010 | 31.733 | 1.00 | 51.69 |
| ATOM | 5730 | C | GLU | 728 | 44.551 | -7.652 | 28.356 | 1.00 | 39.57 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5731 | O | GLU | 728 | 44.852 | -6.605 | 28.933 | 1.00 | 39.30 |
| ATOM | 5732 | N | LEU | 729 | 44.872 | -7.907 | 27.089 | 1.00 | 37.38 |
| ATOM | 5734 | CA | LEU | 729 | 45.655 | -6.977 | 26.274 | 1.00 | 36.74 |
| ATOM | 5735 | CB | LEU | 729 | 46.027 | -7.623 | 24.935 | 1.00 | 35.39 |
| ATOM | 5736 | CG | LEU | 729 | 47.137 | -8.679 | 25.001 | 1.00 | 35.41 |
| ATOM | 5737 | CD1 | LEU | 729 | 47.107 | -9.553 | 23.766 | 1.00 | 35.69 |
| ATOM | 5738 | CD2 | LEU | 729 | 48.505 | -8.017 | 25.174 | 1.00 | 37.72 |
| ATOM | 5739 | C | LEU | 729 | 44.885 | -5.679 | 26.050 | 1.00 | 35.52 |
| ATOM | 5740 | O | LEU | 729 | 45.467 | -4.597 | 25.941 | 1.00 | 33.96 |
| ATOM | 5741 | N | TYR | 730 | 43.565 | -5.779 | 26.000 | 1.00 | 32.90 |
| ATOM | 5743 | CA | TYR | 730 | 42.760 | -4.598 | 25.812 | 1.00 | 32.41 |
| ATOM | 5744 | CB | TYR | 730 | 41.335 | -4.981 | 25.398 | 1.00 | 32.16 |
| ATOM | 5745 | CG | TYR | 730 | 40.445 | -3.787 | 25.172 | 1.00 | 34.93 |
| ATOM | 5746 | CD1 | TYR | 730 | 40.769 | -2.827 | 24.203 | 1.00 | 32.49 |
| ATOM | 5747 | CE1 | TYR | 730 | 39.962 | -1.716 | 23.994 | 1.00 | 32.80 |
| ATOM | 5748 | CD2 | TYR | 730 | 39.282 | -3.605 | 25.931 | 1.00 | 33.45 |
| ATOM | 5749 | CE2 | TYR | 730 | 38.465 | -2.496 | 25.728 | 1.00 | 34.81 |
| ATOM | 5750 | CZ | TYR | 730 | 38.814 | -1.557 | 24.756 | 1.00 | 34.06 |
| ATOM | 5751 | OH | TYR | 730 | 38.009 | -0.465 | 24.551 | 1.00 | 36.66 |
| ATOM | 5753 | C | TYR | 730 | 42.767 | -3.788 | 27.107 | 1.00 | 33.48 |
| ATOM | 5754 | O | TYR | 730 | 42.837 | -2.558 | 27.083 | 1.00 | 34.94 |
| ATOM | 5755 | N | MET | 731 | 42.698 | -4.466 | 28.248 | 1.00 | 35.29 |
| ATOM | 5757 | CA | MET | 731 | 42.724 | -3.755 | 29.525 | 1.00 | 38.38 |
| ATOM | 5758 | CB | MET | 731 | 42.465 | -4.709 | 30.690 | 1.00 | 42.01 |
| ATOM | 5759 | CG | MET | 731 | 41.048 | -5.264 | 30.702 | 1.00 | 53.67 |
| ATOM | 5760 | SD | MET | 731 | 39.785 | -3.965 | 30.830 | 1.00 | 62.97 |
| ATOM | 5761 | CE | MET | 731 | 39.828 | -3.688 | 32.641 | 1.00 | 61.83 |
| ATOM | 5762 | C | MET | 731 | 44.073 | -3.049 | 29.670 | 1.00 | 34.52 |
| ATOM | 5763 | O | MET | 731 | 44.160 | -1.958 | 30.232 | 1.00 | 33.23 |
| ATOM | 5764 | N | MET | 732 | 45.118 | -3.669 | 29.134 | 1.00 | 33.93 |
| ATOM | 5766 | CA | MET | 732 | 46.445 | -3.065 | 29.168 | 1.00 | 36.26 |
| ATOM | 5767 | CB | MET | 732 | 47.506 | -3.995 | 28.565 | 1.00 | 35.56 |
| ATOM | 5768 | CG | MET | 732 | 48.935 | -3.418 | 28.643 | 1.00 | 35.26 |
| ATOM | 5769 | SD | MET | 732 | 50.186 | -4.522 | 28.001 | 1.00 | 30.46 |
| ATOM | 5770 | CE | MET | 732 | 50.480 | -5.562 | 29.415 | 1.00 | 26.88 |
| ATOM | 5771 | C | MET | 732 | 46.369 | -1.750 | 28.389 | 1.00 | 34.75 |
| ATOM | 5772 | O | MET | 732 | 46.827 | -0.722 | 28.873 | 1.00 | 35.49 |
| ATOM | 5773 | N | MET | 733 | 45.741 | -1.774 | 27.213 | 1.00 | 34.63 |
| ATOM | 5775 | CA | MET | 733 | 45.571 | -0.566 | 26.413 | 1.00 | 32.79 |
| ATOM | 5776 | CB | MET | 733 | 44.787 | -0.853 | 25.130 | 1.00 | 33.16 |
| ATOM | 5777 | CG | MET | 733 | 45.544 | -1.601 | 24.047 | 1.00 | 32.32 |
| ATOM | 5778 | SD | MET | 733 | 44.421 | -1.990 | 22.670 | 1.00 | 35.66 |
| ATOM | 5779 | CE | MET | 733 | 45.155 | -3.496 | 22.068 | 1.00 | 29.47 |
| ATOM | 5780 | C | MET | 733 | 44.789 | 0.452 | 27.229 | 1.00 | 33.94 |
| ATOM | 5781 | O | MET | 733 | 45.176 | 1.619 | 27.318 | 1.00 | 35.72 |
| ATOM | 5782 | N | ARG | 734 | 43.679 | 0.018 | 27.818 | 1.00 | 33.73 |
| ATOM | 5784 | CA | ARG | 734 | 42.854 | 0.913 | 28.621 | 1.00 | 33.41 |
| ATOM | 5785 | CB | ARG | 734 | 41.586 | 0.197 | 29.095 | 1.00 | 33.42 |
| ATOM | 5786 | CG | ARG | 734 | 40.726 | -0.335 | 27.950 | 1.00 | 34.26 |
| ATOM | 5787 | CD | ARG | 734 | 40.256 | 0.783 | 27.043 | 1.00 | 37.70 |
| ATOM | 5788 | NE | ARG | 734 | 39.416 | 1.745 | 27.750 | 1.00 | 43.98 |
| ATOM | 5790 | CZ | ARG | 734 | 38.092 | 1.661 | 27.844 | 1.00 | 46.43 |
| ATOM | 5791 | NH1 | ARG | 734 | 37.439 | 0.660 | 27.268 | 1.00 | 48.63 |
| ATOM | 5794 | NH2 | ARG | 734 | 37.420 | 2.571 | 28.530 | 1.00 | 44.65 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5797 | C | ARG | 734 | 43.660 | 1.458 | 29.793 | 1.00 | 32.12 |
| ATOM | 5798 | O | ARG | 734 | 43.492 | 2.610 | 30.180 | 1.00 | 35.37 |
| ATOM | 5799 | N | ASP | 735 | 44.566 | 0.646 | 30.327 | 1.00 | 33.75 |
| ATOM | 5801 | CA | ASP | 735 | 45.438 | 1.076 | 31.433 | 1.00 | 36.72 |
| ATOM | 5802 | CB | ASP | 735 | 46.379 | -0.055 | 31.857 | 1.00 | 42.71 |
| ATOM | 5803 | CG | ASP | 735 | 45.722 | -1.052 | 32.774 | 1.00 | 47.31 |
| ATOM | 5804 | OD1 | ASP | 735 | 46.124 | -2.241 | 32.720 | 1.00 | 50.99 |
| ATOM | 5805 | OD2 | ASP | 735 | 44.824 | -0.646 | 33.552 | 1.00 | 48.45 |
| ATOM | 5806 | C | ASP | 735 | 46.291 | 2.251 | 30.972 | 1.00 | 34.25 |
| ATOM | 5807 | O | ASP | 735 | 46.376 | 3.286 | 31.648 | 1.00 | 34.31 |
| ATOM | 5808 | N | CYS | 736 | 46.927 | 2.064 | 29.816 | 1.00 | 31.85 |
| ATOM | 5810 | CA | CYS | 736 | 47.780 | 3.077 | 29.204 | 1.00 | 29.93 |
| ATOM | 5811 | CB | CYS | 736 | 48.413 | 2.545 | 27.921 | 1.00 | 24.97 |
| ATOM | 5812 | SG | CYS | 736 | 49.504 | 1.159 | 28.180 | 1.00 | 31.35 |
| ATOM | 5813 | C | CYS | 736 | 46.994 | 4.325 | 28.885 | 1.00 | 31.62 |
| ATOM | 5814 | O | CYS | 736 | 47.562 | 5.416 | 28.823 | 1.00 | 30.73 |
| ATOM | 5815 | N | TRP | 737 | 45.680 | 4.174 | 28.711 | 1.00 | 35.03 |
| ATOM | 5817 | CA | TRP | 737 | 44.812 | 5.308 | 28.395 | 1.00 | 36.35 |
| ATOM | 5818 | CB | TRP | 737 | 43.808 | 4.927 | 27.297 | 1.00 | 36.43 |
| ATOM | 5819 | CG | TRP | 737 | 44.451 | 4.487 | 26.010 | 1.00 | 34.34 |
| ATOM | 5820 | CD2 | TRP | 737 | 43.914 | 3.565 | 25.052 | 1.00 | 34.81 |
| ATOM | 5821 | CE2 | TRP | 737 | 44.852 | 3.461 | 23.999 | 1.00 | 33.92 |
| ATOM | 5822 | CE3 | TRP | 737 | 42.730 | 2.816 | 24.980 | 1.00 | 33.06 |
| ATOM | 5823 | CD1 | TRP | 737 | 45.659 | 4.890 | 25.514 | 1.00 | 35.19 |
| ATOM | 5824 | NE1 | TRP | 737 | 45.907 | 4.279 | 24.309 | 1.00 | 35.00 |
| ATOM | 5826 | CZ2 | TRP | 737 | 44.644 | 2.633 | 22.886 | 1.00 | 33.45 |
| ATOM | 5827 | CZ3 | TRP | 737 | 42.527 | 1.991 | 23.876 | 1.00 | 32.92 |
| ATOM | 5828 | CH2 | TRP | 737 | 43.480 | 1.909 | 22.844 | 1.00 | 30.45 |
| ATOM | 5829 | C | TRP | 737 | 44.080 | 5.895 | 29.609 | 1.00 | 37.23 |
| ATOM | 5830 | O | TRP | 737 | 43.047 | 6.551 | 29.474 | 1.00 | 37.44 |
| ATOM | 5831 | N | HIS | 738 | 44.624 | 5.681 | 30.798 | 1.00 | 41.45 |
| ATOM | 5833 | CA | HIS | 738 | 44.006 | 6.208 | 32.008 | 1.00 | 41.52 |
| ATOM | 5834 | CB | HIS | 738 | 44.675 | 5.635 | 33.258 | 1.00 | 41.23 |
| ATOM | 5835 | CG | HIS | 738 | 43.925 | 5.924 | 34.522 | 1.00 | 43.31 |
| ATOM | 5836 | CD2 | HIS | 738 | 43.618 | 7.096 | 35.126 | 1.00 | 41.58 |
| ATOM | 5837 | ND1 | HIS | 738 | 43.338 | 4.935 | 35.279 | 1.00 | 44.22 |
| ATOM | 5839 | CE1 | HIS | 738 | 42.693 | 5.487 | 36.294 | 1.00 | 46.62 |
| ATOM | 5840 | NE2 | HIS | 738 | 42.848 | 6.798 | 36.223 | 1.00 | 43.99 |
| ATOM | 5842 | C | HIS | 738 | 44.118 | 7.726 | 32.015 | 1.00 | 41.75 |
| ATOM | 5843 | O | HIS | 738 | 45.179 | 8.268 | 31.731 | 1.00 | 40.84 |
| ATOM | 5844 | N | ALA | 739 | 43.025 | 8.405 | 32.352 | 1.00 | 42.47 |
| ATOM | 5846 | CA | ALA | 739 | 43.004 | 9.873 | 32.398 | 1.00 | 44.58 |
| ATOM | 5847 | CB | ALA | 739 | 41.629 | 10.361 | 32.825 | 1.00 | 48.19 |
| ATOM | 5848 | C | ALA | 739 | 44.081 | 10.467 | 33.317 | 1.00 | 45.12 |
| ATOM | 5849 | O | ALA | 739 | 44.653 | 11.510 | 33.020 | 1.00 | 45.66 |
| ATOM | 5850 | N | VAL | 740 | 44.262 | 9.852 | 34.481 | 1.00 | 46.64 |
| ATOM | 5852 | CA | VAL | 740 | 45.278 | 10.273 | 35.453 | 1.00 | 46.78 |
| ATOM | 5853 | CB | VAL | 740 | 44.867 | 9.893 | 36.888 | 1.00 | 47.74 |
| ATOM | 5854 | CG1 | VAL | 740 | 45.919 | 10.372 | 37.890 | 1.00 | 49.35 |
| ATOM | 5855 | CG2 | VAL | 740 | 43.515 | 10.495 | 37.211 | 1.00 | 47.89 |
| ATOM | 5856 | C | VAL | 740 | 46.601 | 9.573 | 35.121 | 1.00 | 45.24 |
| ATOM | 5857 | O | VAL | 740 | 46.754 | 8.362 | 35.347 | 1.00 | 45.01 |
| ATOM | 5858 | N | PRO | 741 | 47.588 | 10.335 | 34.637 | 1.00 | 43.46 |
| ATOM | 5859 | CD | PRO | 741 | 47.536 | 11.794 | 34.437 | 1.00 | 43.51 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5860 | CA | PRO | 741 | 48.905 | 9.804 | 34.266 | 1.00 | 46.22 |
| ATOM | 5861 | CB | PRO | 741 | 49.701 | 11.070 | 33.942 | 1.00 | 45.32 |
| ATOM | 5862 | CG | PRO | 741 | 48.632 | 12.010 | 33.426 | 1.00 | 42.81 |
| ATOM | 5863 | C | PRO | 741 | 49.588 | 8.936 | 35.328 | 1.00 | 47.45 |
| ATOM | 5864 | O | PRO | 741 | 50.245 | 7.950 | 34.994 | 1.00 | 45.12 |
| ATOM | 5865 | N | SER | 742 | 49.394 | 9.280 | 36.601 | 1.00 | 48.78 |
| ATOM | 5867 | CA | SER | 742 | 49.994 | 8.532 | 37.703 | 1.00 | 48.76 |
| ATOM | 5868 | CB | SER | 742 | 49.845 | 9.317 | 39.012 | 1.00 | 51.11 |
| ATOM | 5869 | OG | SER | 742 | 48.482 | 9.488 | 39.373 | 1.00 | 53.50 |
| ATOM | 5871 | C | SER | 742 | 49.376 | 7.150 | 37.867 | 1.00 | 47.77 |
| ATOM | 5872 | O | SER | 742 | 49.932 | 6.283 | 38.539 | 1.00 | 47.31 |
| ATOM | 5873 | N | GLN | 743 | 48.199 | 6.962 | 37.284 | 1.00 | 47.57 |
| ATOM | 5875 | CA | GLN | 743 | 47.511 | 5.689 | 37.384 | 1.00 | 47.14 |
| ATOM | 5876 | CB | GLN | 743 | 46.004 | 5.918 | 37.531 | 1.00 | 50.16 |
| ATOM | 5877 | CG | GLN | 743 | 45.438 | 5.447 | 38.871 | 1.00 | 54.69 |
| ATOM | 5878 | CD | GLN | 743 | 46.239 | 5.964 | 40.051 | 1.00 | 57.62 |
| ATOM | 5879 | OE1 | GLN | 743 | 46.898 | 5.196 | 40.749 | 1.00 | 59.09 |
| ATOM | 5880 | NE2 | GLN | 743 | 46.202 | 7.277 | 40.268 | 1.00 | 59.45 |
| ATOM | 5883 | C | GLN | 743 | 47.816 | 4.774 | 36.212 | 1.00 | 44.41 |
| ATOM | 5884 | O | GLN | 743 | 47.365 | 3.627 | 36.182 | 1.00 | 44.39 |
| ATOM | 5885 | N | ARG | 744 | 48.515 | 5.305 | 35.212 | 1.00 | 42.87 |
| ATOM | 5887 | CA | ARG | 744 | 48.902 | 4.506 | 34.046 | 1.00 | 41.45 |
| ATOM | 5888 | CB | ARG | 744 | 49.350 | 5.397 | 32.883 | 1.00 | 37.34 |
| ATOM | 5889 | CG | ARG | 744 | 48.316 | 6.380 | 32.412 | 1.00 | 32.30 |
| ATOM | 5890 | CD | ARG | 744 | 48.854 | 7.207 | 31.270 | 1.00 | 31.37 |
| ATOM | 5891 | NE | ARG | 744 | 47.921 | 8.276 | 30.946 | 1.00 | 36.76 |
| ATOM | 5893 | CZ | ARG | 744 | 48.271 | 9.492 | 30.543 | 1.00 | 39.88 |
| ATOM | 5894 | NH1 | ARG | 744 | 49.553 | 9.813 | 30.399 | 1.00 | 39.94 |
| ATOM | 5897 | NH2 | ARG | 744 | 47.330 | 10.404 | 30.322 | 1.00 | 39.12 |
| ATOM | 5900 | C | ARG | 744 | 50.068 | 3.616 | 34.471 | 1.00 | 41.40 |
| ATOM | 5901 | O | ARG | 744 | 50.813 | 3.945 | 35.405 | 1.00 | 42.84 |
| ATOM | 5902 | N | PRO | 745 | 50.203 | 2.441 | 33.849 | 1.00 | 40.11 |
| ATOM | 5903 | CD | PRO | 745 | 49.345 | 1.739 | 32.876 | 1.00 | 39.91 |
| ATOM | 5904 | CA | PRO | 745 | 51.332 | 1.607 | 34.266 | 1.00 | 38.58 |
| ATOM | 5905 | CB | PRO | 745 | 51.019 | 0.261 | 33.605 | 1.00 | 37.46 |
| ATOM | 5906 | CG | PRO | 745 | 50.250 | 0.645 | 32.377 | 1.00 | 37.41 |
| ATOM | 5907 | C | PRO | 745 | 52.640 | 2.202 | 33.750 | 1.00 | 37.73 |
| ATOM | 5908 | O | PRO | 745 | 52.634 | 3.027 | 32.835 | 1.00 | 37.71 |
| ATOM | 5909 | N | THR | 746 | 53.753 | 1.843 | 34.373 | 1.00 | 35.90 |
| ATOM | 5911 | CA | THR | 746 | 55.050 | 2.328 | 33.913 | 1.00 | 34.77 |
| ATOM | 5912 | CB | THR | 746 | 56.085 | 2.380 | 35.075 | 1.00 | 33.85 |
| ATOM | 5913 | OG1 | THR | 746 | 56.296 | 1.059 | 35.602 | 1.00 | 33.92 |
| ATOM | 5915 | CG2 | THR | 746 | 55.605 | 3.302 | 36.177 | 1.00 | 32.17 |
| ATOM | 5916 | C | THR | 746 | 55.544 | 1.327 | 32.870 | 1.00 | 32.69 |
| ATOM | 5917 | O | THR | 746 | 55.026 | 0.213 | 32.795 | 1.00 | 31.56 |
| ATOM | 5918 | N | PHE | 747 | 56.538 | 1.708 | 32.066 | 1.00 | 34.04 |
| ATOM | 5920 | CA | PHE | 747 | 57.093 | 0.782 | 31.083 | 1.00 | 31.74 |
| ATOM | 5921 | CB | PHE | 747 | 58.121 | 1.472 | 30.193 | 1.00 | 30.55 |
| ATOM | 5922 | CG | PHE | 747 | 57.504 | 2.287 | 29.096 | 1.00 | 29.40 |
| ATOM | 5923 | CD1 | PHE | 747 | 56.772 | 1.666 | 28.092 | 1.00 | 28.24 |
| ATOM | 5924 | CD2 | PHE | 747 | 57.609 | 3.667 | 29.091 | 1.00 | 27.50 |
| ATOM | 5925 | CE1 | PHE | 747 | 56.170 | 2.407 | 27.100 | 1.00 | 24.35 |
| ATOM | 5926 | CE2 | PHE | 747 | 57.001 | 4.413 | 28.091 | 1.00 | 29.27 |
| ATOM | 5927 | CZ | PHE | 747 | 56.276 | 3.776 | 27.103 | 1.00 | 25.73 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5928 | C | PHE | 747 | 57.714 | -0.413 | 31.782 | 1.00 | 31.92 |
| ATOM | 5929 | O | PHE | 747 | 57.727 | -1.514 | 31.243 | 1.00 | 32.46 |
| ATOM | 5930 | N | LYS | 748 | 58.233 | -0.199 | 32.986 | 1.00 | 33.47 |
| ATOM | 5932 | CA | LYS | 748 | 58.816 | -1.302 | 33.733 | 1.00 | 35.57 |
| ATOM | 5933 | CB | LYS | 748 | 59.468 | -0.800 | 35.026 | 1.00 | 39.42 |
| ATOM | 5934 | CG | LYS | 748 | 60.083 | -1.923 | 35.861 | 1.00 | 46.49 |
| ATOM | 5935 | CD | LYS | 748 | 60.817 | -1.407 | 37.103 | 1.00 | 50.69 |
| ATOM | 5936 | CE | LYS | 748 | 61.253 | -2.574 | 37.999 | 1.00 | 52.57 |
| ATOM | 5937 | NZ | LYS | 748 | 62.072 | -2.129 | 39.155 | 1.00 | 56.45 |
| ATOM | 5941 | C | LYS | 748 | 57.700 | -2.318 | 34.028 | 1.00 | 35.58 |
| ATOM | 5942 | O | LYS | 748 | 57.898 | -3.526 | 33.871 | 1.00 | 34.72 |
| ATOM | 5943 | N | GLN | 749 | 56.522 | -1.818 | 34.411 | 1.00 | 35.59 |
| ATOM | 5945 | CA | GLN | 749 | 55.369 | -2.684 | 34.692 | 1.00 | 38.20 |
| ATOM | 5946 | CB | GLN | 749 | 54.154 | -1.872 | 35.162 | 1.00 | 42.73 |
| ATOM | 5947 | CG | GLN | 749 | 54.264 | -1.171 | 36.499 | 1.00 | 49.30 |
| ATOM | 5948 | CD | GLN | 749 | 53.060 | -0.282 | 36.761 | 1.00 | 53.13 |
| ATOM | 5949 | OE1 | GLN | 749 | 53.194 | 0.915 | 37.023 | 1.00 | 52.71 |
| ATOM | 5950 | NE2 | GLN | 749 | 51.873 | -0.856 | 36.644 | 1.00 | 58.54 |
| ATOM | 5953 | C | GLN | 749 | 54.954 | -3.392 | 33.409 | 1.00 | 36.16 |
| ATOM | 5954 | O | GLN | 749 | 54.745 | -4.605 | 33.393 | 1.00 | 36.67 |
| ATOM | 5955 | N | LEU | 750 | 54.801 | -2.609 | 32.342 | 1.00 | 35.83 |
| ATOM | 5957 | CA | LEU | 750 | 54.381 | -3.117 | 31.037 | 1.00 | 34.49 |
| ATOM | 5958 | CB | LEU | 750 | 54.324 | -1.988 | 30.004 | 1.00 | 32.49 |
| ATOM | 5959 | CG | LEU | 750 | 53.206 | -0.958 | 30.188 | 1.00 | 31.94 |
| ATOM | 5960 | CD1 | LEU | 750 | 53.411 | 0.230 | 29.267 | 1.00 | 30.45 |
| ATOM | 5961 | CD2 | LEU | 750 | 51.859 | -1.610 | 29.933 | 1.00 | 29.30 |
| ATOM | 5962 | C | LEU | 750 | 55.294 | -4.214 | 30.559 | 1.00 | 33.87 |
| ATOM | 5963 | O | LEU | 750 | 54.828 | -5.208 | 30.027 | 1.00 | 34.72 |
| ATOM | 5964 | N | VAL | 751 | 56.598 | -4.038 | 30.759 | 1.00 | 36.12 |
| ATOM | 5966 | CA | VAL | 751 | 57.585 | -5.045 | 30.363 | 1.00 | 34.50 |
| ATOM | 5967 | CB | VAL | 751 | 59.054 | -4.532 | 30.559 | 1.00 | 31.96 |
| ATOM | 5968 | CG1 | VAL | 751 | 60.052 | -5.646 | 30.308 | 1.00 | 30.24 |
| ATOM | 5969 | CG2 | VAL | 751 | 59.342 | -3.386 | 29.604 | 1.00 | 28.02 |
| ATOM | 5970 | C | VAL | 751 | 57.349 | -6.321 | 31.182 | 1.00 | 36.11 |
| ATOM | 5971 | O | VAL | 751 | 57.333 | -7.422 | 30.638 | 1.00 | 36.45 |
| ATOM | 5972 | N | GLU | 752 | 57.107 | -6.165 | 32.479 | 1.00 | 37.83 |
| ATOM | 5974 | CA | GLU | 752 | 56.869 | -7.326 | 33.331 | 1.00 | 41.47 |
| ATOM | 5975 | CB | GLU | 752 | 56.800 | -6.910 | 34.804 | 1.00 | 43.03 |
| ATOM | 5976 | CG | GLU | 752 | 58.122 | -6.305 | 35.263 | 1.00 | 52.52 |
| ATOM | 5977 | CD | GLU | 752 | 58.251 | -6.176 | 36.761 | 1.00 | 57.18 |
| ATOM | 5978 | OE1 | GLU | 752 | 58.600 | -5.068 | 37.233 | 1.00 | 58.11 |
| ATOM | 5979 | OE2 | GLU | 752 | 58.032 | -7.191 | 37.461 | 1.00 | 61.59 |
| ATOM | 5980 | C | GLU | 752 | 55.623 | -8.097 | 32.890 | 1.00 | 40.16 |
| ATOM | 5981 | O | GLU | 752 | 55.689 | -9.308 | 32.642 | 1.00 | 39.75 |
| ATOM | 5982 | N | ASP | 753 | 54.524 | -7.376 | 32.696 | 1.00 | 40.06 |
| ATOM | 5984 | CA | ASP | 753 | 53.275 | -7.982 | 32.264 | 1.00 | 39.73 |
| ATOM | 5985 | CB | ASP | 753 | 52.157 | -6.947 | 32.247 | 1.00 | 41.00 |
| ATOM | 5986 | CG | ASP | 753 | 51.668 | -6.591 | 33.640 | 1.00 | 45.17 |
| ATOM | 5987 | OD1 | ASP | 753 | 51.753 | -7.468 | 34.543 | 1.00 | 49.78 |
| ATOM | 5988 | OD2 | ASP | 753 | 51.210 | -5.439 | 33.829 | 1.00 | 45.51 |
| ATOM | 5989 | C | ASP | 753 | 53.396 | -8.595 | 30.890 | 1.00 | 39.64 |
| ATOM | 5990 | O | ASP | 753 | 52.955 | -9.720 | 30.674 | 1.00 | 41.84 |
| ATOM | 5991 | N | LEU | 754 | 53.998 | -7.861 | 29.960 | 1.00 | 37.75 |
| ATOM | 5993 | CA | LEU | 754 | 54.161 | -8.358 | 28.603 | 1.00 | 38.16 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5994 | CB | LEU | 754 | 54.664 | -7.261 | 27.664 | 1.00 | 36.95 |
| ATOM | 5995 | CG | LEU | 754 | 53.552 | -6.270 | 27.307 | 1.00 | 36.64 |
| ATOM | 5996 | CD1 | LEU | 754 | 54.141 | -5.062 | 26.590 | 1.00 | 34.02 |
| ATOM | 5997 | CD2 | LEU | 754 | 52.459 | -6.968 | 26.465 | 1.00 | 34.13 |
| ATOM | 5998 | C | LEU | 754 | 55.070 | -9.561 | 28.571 | 1.00 | 38.46 |
| ATOM | 5999 | O | LEU | 754 | 54.905 | -10.451 | 27.740 | 1.00 | 39.95 |
| ATOM | 6000 | N | ASP | 755 | 56.014 | -9.602 | 29.502 | 1.00 | 39.19 |
| ATOM | 6002 | CA | ASP | 755 | 56.930 | -10.728 | 29.594 | 1.00 | 40.87 |
| ATOM | 6003 | CB | ASP | 755 | 57.956 | -10.462 | 30.696 | 1.00 | 45.11 |
| ATOM | 6004 | CG | ASP | 755 | 59.128 | -11.415 | 30.652 | 1.00 | 48.64 |
| ATOM | 6005 | OD1 | ASP | 755 | 59.759 | -11.612 | 31.711 | 1.00 | 54.27 |
| ATOM | 6006 | OD2 | ASP | 755 | 59.432 | -11.954 | 29.565 | 1.00 | 51.46 |
| ATOM | 6007 | C | ASP | 755 | 56.082 | -11.952 | 29.947 | 1.00 | 40.67 |
| ATOM | 6008 | O | ASP | 755 | 56.152 | -12.996 | 29.289 | 1.00 | 38.49 |
| ATOM | 6009 | N | ARG | 756 | 55.232 | -11.771 | 30.955 | 1.00 | 40.06 |
| ATOM | 6011 | CA | ARG | 756 | 54.340 | -12.817 | 31.437 | 1.00 | 40.07 |
| ATOM | 6012 | CB | ARG | 756 | 53.573 | -12.316 | 32.661 | 1.00 | 40.24 |
| ATOM | 6013 | CG | ARG | 756 | 52.435 | -13.217 | 33.138 | 1.00 | 42.12 |
| ATOM | 6014 | CD | ARG | 756 | 51.791 | -12.631 | 34.389 | 1.00 | 42.33 |
| ATOM | 6015 | NE | ARG | 756 | 51.353 | -11.247 | 34.186 | 1.00 | 46.68 |
| ATOM | 6017 | CZ | ARG | 756 | 50.295 | -10.891 | 33.460 | 1.00 | 48.17 |
| ATOM | 6018 | NH1 | ARG | 756 | 49.549 | -11.818 | 32.866 | 1.00 | 46.64 |
| ATOM | 6021 | NH2 | ARG | 756 | 49.998 | -9.605 | 33.305 | 1.00 | 48.92 |
| ATOM | 6024 | C | ARG | 756 | 53.362 | -13.275 | 30.364 | 1.00 | 40.19 |
| ATOM | 6025 | O | ARG | 756 | 53.247 | -14.469 | 30.110 | 1.00 | 42.24 |
| ATOM | 6026 | N | ILE | 757 | 52.688 | -12.327 | 29.717 | 1.00 | 38.18 |
| ATOM | 6028 | CA | ILE | 757 | 51.706 | -12.649 | 28.683 | 1.00 | 38.40 |
| ATOM | 6029 | CB | ILE | 757 | 50.952 | -11.382 | 28.187 | 1.00 | 36.55 |
| ATOM | 6030 | CG2 | ILE | 757 | 49.952 | -11.758 | 27.105 | 1.00 | 34.67 |
| ATOM | 6031 | CG1 | ILE | 757 | 50.216 | -10.726 | 29.364 | 1.00 | 34.65 |
| ATOM | 6032 | CD1 | ILE | 757 | 49.554 | -9.423 | 29.048 | 1.00 | 36.49 |
| ATOM | 6033 | C | ILE | 757 | 52.301 | -13.400 | 27.500 | 1.00 | 39.19 |
| ATOM | 6034 | O | ILE | 757 | 51.709 | -14.360 | 27.025 | 1.00 | 39.66 |
| ATOM | 6035 | N | VAL | 758 | 53.492 | -12.996 | 27.061 | 1.00 | 42.36 |
| ATOM | 6037 | CA | VAL | 758 | 54.161 | -13.645 | 25.937 | 1.00 | 43.15 |
| ATOM | 6038 | CB | VAL | 758 | 55.582 | -13.052 | 25.682 | 1.00 | 41.72 |
| ATOM | 6039 | CG1 | VAL | 758 | 56.308 | -13.855 | 24.621 | 1.00 | 41.57 |
| ATOM | 6040 | CG2 | VAL | 758 | 55.491 | -11.619 | 25.229 | 1.00 | 40.06 |
| ATOM | 6041 | C | VAL | 758 | 54.299 | -15.133 | 26.231 | 1.00 | 47.11 |
| ATOM | 6042 | O | VAL | 758 | 54.045 | -15.971 | 25.369 | 1.00 | 48.62 |
| ATOM | 6043 | N | ALA | 759 | 54.695 | -15.446 | 27.464 | 1.00 | 49.64 |
| ATOM | 6045 | CA | ALA | 759 | 54.879 | -16.820 | 27.908 | 1.00 | 51.35 |
| ATOM | 6046 | CB | ALA | 759 | 55.423 | -16.830 | 29.317 | 1.00 | 50.11 |
| ATOM | 6047 | C | ALA | 759 | 53.568 | -17.598 | 27.850 | 1.00 | 54.72 |
| ATOM | 6048 | O | ALA | 759 | 53.520 | -18.717 | 27.348 | 1.00 | 58.64 |
| ATOM | 6049 | N | LEU | 760 | 52.496 | -16.983 | 28.329 | 1.00 | 54.84 |
| ATOM | 6051 | CA | LEU | 760 | 51.194 | -17.628 | 28.343 | 1.00 | 55.87 |
| ATOM | 6052 | CB | LEU | 760 | 50.330 | -17.034 | 29.459 | 1.00 | 56.85 |
| ATOM | 6053 | CG | LEU | 760 | 50.875 | -17.165 | 30.885 | 1.00 | 56.80 |
| ATOM | 6054 | CD1 | LEU | 760 | 49.991 | -16.392 | 31.849 | 1.00 | 56.78 |
| ATOM | 6055 | CD2 | LEU | 760 | 50.959 | -18.631 | 31.289 | 1.00 | 57.78 |
| ATOM | 6056 | C | LEU | 760 | 50.454 | -17.546 | 27.013 | 1.00 | 57.36 |
| ATOM | 6057 | O | LEU | 760 | 49.262 | -17.859 | 26.944 | 1.00 | 57.65 |
| ATOM | 6058 | N | THR | 761 | 51.151 | -17.134 | 25.956 | 1.00 | 58.71 |

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ATOM   6060  CA   THR   761     50.541  -17.025   24.630  1.00  59.04
ATOM   6061  CB   THR   761     50.839  -15.657   23.971  1.00  56.72
ATOM   6062  OG1  THR   761     50.287  -14.610   24.775  1.00  56.53
ATOM   6064  CG2  THR   761     50.213  -15.584   22.590  1.00  53.81
ATOM   6065  C    THR   761     51.049  -18.138   23.721  1.00  60.44
ATOM   6066  O    THR   761     52.255  -18.295   23.530  1.00  61.40
ATOM   6067  SG   CYS   1603    18.474   -8.976   20.202  0.50  37.82  PRT2
ATOM   6068  CG   MET   534     69.311   12.109   23.281  0.50  36.25  PRT2
ATOM   6069  SD   MET   534     69.286   12.958   24.867  0.50  42.66  PRT2
ATOM   6070  CE   MET   534     70.539   12.083   25.804  0.50  43.27  PRT2
ATOM   6071  SG   CYS   603     56.046   -7.949   16.446  0.50  36.47  PRT2
ATOM   2676  OH2  TIP3  1       71.794   25.061    2.660  1.00  24.53
ATOM   2679  OH2  TIP3  2       39.750    3.992   15.898  1.00  39.62
ATOM   2682  OH2  TIP3  3       83.809   19.717   10.596  1.00  28.26
ATOM   2685  OH2  TIP3  4       83.630   20.056    7.685  1.00  26.19
ATOM   2688  OH2  TIP3  5       75.073   16.616    6.785  1.00  26.48
ATOM   2691  OH2  TIP3  6       86.549   19.594    9.502  1.00  33.65
ATOM   2694  OH2  TIP3  7       51.913   11.060   24.263  1.00  35.55
ATOM   2697  OH2  TIP3  8       55.093    9.421   22.524  1.00  26.63
ATOM   2700  OH2  TIP3  9       57.161    4.614   32.443  1.00  29.69
ATOM   2703  OH2  TIP3  10      52.169    4.735   13.281  1.00  22.61
ATOM   2706  OH2  TIP3  11      41.110    5.543   22.764  1.00  41.60
ATOM   2709  OH2  TIP3  12      45.145    8.857   21.555  1.00  36.99
ATOM   2712  OH2  TIP3  13      64.465   -2.607   28.883  1.00  30.17
ATOM   2715  OH2  TIP3  14      76.944   13.287   23.954  1.00  32.94
ATOM   2718  OH2  TIP3  15      79.062   17.048   18.200  1.00  51.65
ATOM   2721  OH2  TIP3  16      83.066   11.657   15.958  1.00  25.12
ATOM   2724  OH2  TIP3  17      13.957   -9.951    0.095  1.00  26.02
ATOM   2727  OH2  TIP3  18      38.359   -0.001    5.000  1.00  37.43
ATOM   2730  OH2  TIP3  19       5.442    2.705   19.077  1.00  29.46
ATOM   2733  OH2  TIP3  20      27.008    6.166    4.885  1.00  25.05
ATOM   2736  OH2  TIP3  21      34.242   -1.725   16.911  1.00  52.12
ATOM   2739  OH2  TIP3  22      20.167    2.428   27.681  1.00  42.69
ATOM   2742  OH2  TIP3  23      50.794  -11.834   38.045  1.00  60.16
ATOM   2745  OH2  TIP3  24      17.261   -5.993   -1.757  1.00  25.88
ATOM   2748  OH2  TIP3  25      27.516    7.803   15.070  1.00  39.33
ATOM   2751  OH2  TIP3  26      31.574    0.146    6.684  1.00  35.78
ATOM   2754  OH2  TIP3  27      27.119  -12.972   27.844  1.00  43.66
ATOM   2757  OH2  TIP3  28      28.439  -17.074   13.203  1.00  36.44
ATOM   2760  OH2  TIP3  29      88.706   14.393    7.969  1.00  32.49
ATOM   2763  OH2  TIP3  30      -2.338   -3.424   11.295  1.00  49.20
ATOM   2766  OH2  TIP3  31      35.086   -4.130   18.836  1.00  37.83
ATOM   2769  OH2  TIP3  32      80.455   17.922    9.507  1.00  23.69
ATOM   2772  OH2  TIP3  33       5.538    3.619   10.835  1.00  29.13
ATOM   2775  OH2  TIP3  34     -10.685    5.290   11.288  1.00  24.40
ATOM   2778  OH2  TIP3  35      29.210   -8.799   20.241  1.00  46.52
ATOM   2781  OH2  TIP3  36       6.195    3.150   13.803  1.00  31.39
ATOM   2784  OH2  TIP3  37      31.898    2.830    0.154  1.00  40.17
ATOM   2787  OH2  TIP3  38      19.915    2.023   -3.939  1.00  31.34
ATOM   2790  OH2  TIP3  39      62.242    2.604   32.859  1.00  39.67
ATOM   2793  OH2  TIP3  40      21.231   -7.063   -3.900  1.00  23.55
ATOM   2796  OH2  TIP3  41     -15.809    8.838   22.610  1.00  36.02
ATOM   2799  OH2  TIP3  42      40.120    2.154    8.433  1.00  60.62
ATOM   2802  OH2  TIP3  43      19.583   11.128   -0.045  1.00  37.85
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ATOM  2805  OH2  TIP3  44    67.056    9.030   17.389  1.00  29.79
ATOM  2808  OH2  TIP3  45    87.772   18.919   18.595  1.00  48.44
ATOM  2811  OH2  TIP3  46    74.584   17.123    4.200  1.00  39.18
ATOM  2814  OH2  TIP3  47    29.365   16.707   10.560  1.00  34.11
ATOM  2817  OH2  TIP3  48    66.486    6.826   15.051  1.00  32.28
ATOM  2820  OH2  TIP3  49    85.008   21.441    5.731  1.00  23.97
ATOM  2823  OH2  TIP3  50    -4.572    2.912    3.173  1.00  28.05
ATOM  2826  OH2  TIP3  51    19.496    5.141    4.881  1.00  28.88
ATOM  2829  OH2  TIP3  52    67.492    3.490   10.902  1.00  33.57
ATOM  2832  OH2  TIP3  53    34.791    5.413   24.797  1.00  40.16
ATOM  2835  OH2  TIP3  54    34.787  -16.910   13.756  1.00  39.46
ATOM  2838  OH2  TIP3  55    59.972    7.450   27.870  1.00  31.56
ATOM  2841  OH2  TIP3  56    -7.139   -1.696    6.345  1.00  42.00
ATOM  2844  OH2  TIP3  57    54.998   11.953   25.360  1.00  42.05
ATOM  2847  OH2  TIP3  58    68.697    6.686   16.740  1.00  46.12
ATOM  2850  OH2  TIP3  59    73.750   20.885   19.041  1.00  32.26
ATOM  2853  OH2  TIP3  60     3.431   -8.270   -8.218  1.00  31.22
ATOM  2856  OH2  TIP3  61    37.904   10.790    5.612  1.00  33.72
ATOM  2859  OH2  TIP3  62    29.982   -9.545   -1.303  1.00  39.11
ATOM  2862  OH2  TIP3  63    66.918    1.757    8.678  1.00  34.68
ATOM  2865  OH2  TIP3  64    49.117    1.310   12.227  1.00  34.31
ATOM  2868  OH2  TIP3  65    41.246    3.987   29.033  1.00  34.55
ATOM  2871  OH2  TIP3  66    10.755  -12.957    1.167  1.00  42.14
ATOM  2874  OH2  TIP3  67    -1.184   -4.327   21.439  1.00  37.90
ATOM  2877  OH2  TIP3  68    30.349   16.267   13.265  1.00  55.23
ATOM  2880  OH2  TIP3  69     8.111    4.362    3.445  1.00  23.88
ATOM  2883  OH2  TIP3  70    73.131   18.780   22.628  1.00  40.20
ATOM  2886  OH2  TIP3  71    -7.949   -3.409   24.953  1.00  35.49
ATOM  2889  OH2  TIP3  72    66.379   -4.621   28.423  1.00  45.46
ATOM  2892  OH2  TIP3  73    21.506  -20.711    4.815  1.00  52.46
ATOM  2895  OH2  TIP3  74    59.539   -6.865    4.928  1.00  48.87
ATOM  2898  OH2  TIP3  75    16.565  -13.297   -3.008  1.00  51.80
ATOM  2901  OH2  TIP3  76   -15.235    7.385    4.428  1.00  29.13
ATOM  2904  OH2  TIP3  77    32.926    2.785   13.213  1.00  37.62
ATOM  2907  OH2  TIP3  78     0.246   -2.768   10.996  1.00  28.25
ATOM  2910  OH2  TIP3  79    17.495    2.354    5.447  1.00  23.63
ATOM  2913  OH2  TIP3  80     6.336    2.434   21.950  1.00  29.56
ATOM  2916  OH2  TIP3  81    27.374    3.628    6.163  1.00  34.06
ATOM  2919  OH2  TIP3  82    -8.708    6.263    9.522  1.00  30.34
ATOM  2922  OH2  TIP3  83     1.500   -1.935    8.721  1.00  27.61
ATOM  2925  OH2  TIP3  84    -4.825   -3.133    6.984  1.00  33.50
ATOM  2928  OH2  TIP3  85    17.513    2.839    1.966  1.00  24.27
ATOM  2931  OH2  TIP3  86    20.298    3.414    2.920  1.00  26.15
ATOM  2934  OH2  TIP3  87     0.488   -2.158   22.213  1.00  25.95
ATOM  2937  OH2  TIP3  88    19.939   -6.185   -1.553  1.00  19.14
ATOM  2940  OH2  TIP3  89    10.670  -15.654    6.839  1.00  33.36
ATOM  2943  OH2  TIP3  90     4.107  -12.003   11.805  1.00  33.92
ATOM  2946  OH2  TIP3  91     6.238    0.927   -3.342  1.00  23.31
ATOM  2949  OH2  TIP3  92   -13.563    1.438    5.472  1.00  27.86
ATOM  2952  OH2  TIP3  93    15.707   -7.454    0.106  1.00  26.69
ATOM  2955  OH2  TIP3  94    -1.856   -5.393    3.795  1.00  39.91
ATOM  2958  OH2  TIP3  95    12.654    4.928   -4.474  1.00  31.32
ATOM  2961  OH2  TIP3  96    69.774   27.363    2.127  1.00  35.86
ATOM  2964  OH2  TIP3  97    24.636  -13.192    0.040  1.00  48.53
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ATOM   2967  OH2  TIP3  98      60.453   -4.625   33.829   1.00   31.97
ATOM   2970  OH2  TIP3  99      10.513    5.719    3.487   1.00   38.90
ATOM   2973  OH2  TIP3  100     -9.499   -4.011    4.342   1.00   30.61
ATOM   2976  OH2  TIP3  101     73.056   -1.608   10.514   1.00   36.08
ATOM   2979  OH2  TIP3  102     -3.152    5.709   30.608   1.00   29.38
ATOM   2982  OH2  TIP3  103     36.630    0.702   11.792   1.00   47.80
ATOM   2985  OH2  TIP3  104     21.475    6.325   16.924   1.00   24.03
ATOM   2988  OH2  TIP3  105     31.272    0.656   19.432   1.00   53.74
ATOM   2991  OH2  TIP3  106      5.620   -8.417   22.266   1.00   51.90
ATOM   2994  OH2  TIP3  107    -13.144    8.294   17.464   1.00   35.23
ATOM   2997  OH2  TIP3  108     26.680  -10.556   -1.042   1.00   27.83
ATOM   3000  OH2  TIP3  109     24.149    1.846   18.172   1.00   30.90
ATOM   3003  OH2  TIP3  110     -1.943   12.643    3.558   1.00   33.82
ATOM   3006  OH2  TIP3  111     59.560   13.617   33.196   1.00   54.79
ATOM   3009  OH2  TIP3  112      4.351  -10.740    1.991   1.00   37.96
ATOM   3012  OH2  TIP3  113      8.396    2.913    0.958   1.00   29.64
ATOM   3015  OH2  TIP3  114     75.905    1.753   25.812   1.00   38.73
ATOM   3018  OH2  TIP3  115     48.783   15.535   14.189   1.00   35.24
ATOM   3021  OH2  TIP3  116      2.419  -11.312    9.146   1.00   32.85
ATOM   3024  OH2  TIP3  117     83.014   26.360   12.964   1.00   41.83
ATOM   3027  OH2  TIP3  118      8.761   -6.579   -3.252   1.00   42.78
ATOM   3030  OH2  TIP3  119     -8.417    4.493    4.305   1.00   28.32
ATOM   3033  OH2  TIP3  120      7.908  -13.690    8.639   1.00   33.73
ATOM   3036  OH2  TIP3  121     51.437    6.329   10.373   1.00   31.72
ATOM   3039  OH2  TIP3  122     20.660    3.686   15.591   1.00   32.37
ATOM   3042  OH2  TIP3  123     73.039    3.790   20.450   1.00   35.80
ATOM   3045  OH2  TIP3  124      5.155  -11.467   22.590   1.00   45.12
ATOM   3048  OH2  TIP3  125     34.172    2.412   16.576   1.00   41.90
ATOM   3051  OH2  TIP3  126      9.597  -11.905    7.083   1.00   24.83
ATOM   3054  OH2  TIP3  127      8.276    3.860   -1.622   1.00   35.46
ATOM   3057  OH2  TIP3  128     66.282    5.755   12.352   1.00   35.43
ATOM   3060  OH2  TIP3  129      7.377    6.932    2.982   1.00   40.68
ATOM   3063  OH2  TIP3  130     35.832   -1.778    0.201   1.00   34.99
ATOM   3066  OH2  TIP3  131     44.781   10.362   11.064   1.00   42.31
ATOM   3069  OH2  TIP3  132     27.790  -12.638   18.958   1.00   58.71
ATOM   3072  OH2  TIP3  133     45.221   11.540   21.428   1.00   36.75
ATOM   3075  OH2  TIP3  134     57.560  -10.846   14.099   1.00   52.90
ATOM   3078  OH2  TIP3  135     -3.354   15.001   16.515   1.00   37.81
ATOM   3081  OH2  TIP3  136     85.717   11.251    9.062   1.00   35.18
ATOM   3084  OH2  TIP3  137     12.951   -2.469    2.075   1.00   22.07
ATOM   3087  OH2  TIP3  138     75.645    3.486   20.527   1.00   38.01
ATOM   3090  OH2  TIP3  139     13.237    7.412   -2.649   1.00   33.50
ATOM   3093  OH2  TIP3  140     11.262   -9.970    0.974   1.00   26.14
ATOM   3096  OH2  TIP3  141     59.480   10.772   14.098   1.00   52.08
ATOM   3099  OH2  TIP3  142     13.869  -16.121    3.919   1.00   40.06
ATOM   3102  OH2  TIP3  143     -6.407   -3.413   16.641   1.00   44.38
ATOM   3105  OH2  TIP3  144     25.667  -12.645    3.411   1.00   48.28
ATOM   3108  OH2  TIP3  145    -16.282   10.641    6.423   1.00   40.94
ATOM   3111  OH2  TIP3  146     86.637   12.861    7.008   1.00   39.45
ATOM   3114  OH2  TIP3  147     32.082   -4.569    1.892   1.00   27.35
ATOM   3117  OH2  TIP3  148     44.809    7.627   11.670   1.00   35.65
ATOM   3120  OH2  TIP3  149     80.693   12.459   16.523   1.00   37.21
ATOM   3123  OH2  TIP3  150      2.941   -7.118   -1.805   1.00   38.43
ATOM   3126  OH2  TIP3  151     31.794   -6.086   20.704   1.00   42.80
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3129 | OH2 | TIP3 | 152 | 74.770 | -2.683 | 12.398 | 1.00 | 40.40 |
| ATOM | 3132 | OH2 | TIP3 | 153 | 7.731 | 6.640 | -1.037 | 1.00 | 35.61 |
| ATOM | 3135 | OH2 | TIP3 | 154 | 71.617 | 5.599 | 21.838 | 1.00 | 40.14 |
| ATOM | 3138 | OH2 | TIP3 | 155 | 68.113 | -4.968 | 8.886 | 1.00 | 34.38 |
| ATOM | 3141 | OH2 | TIP3 | 156 | 0.042 | -9.364 | 7.055 | 1.00 | 33.08 |
| ATOM | 3144 | OH2 | TIP3 | 157 | 68.020 | 18.352 | 10.995 | 1.00 | 34.76 |
| ATOM | 3147 | OH2 | TIP3 | 158 | 3.795 | 8.550 | 4.533 | 1.00 | 34.69 |
| ATOM | 3150 | OH2 | TIP3 | 159 | 52.106 | 11.746 | 18.410 | 1.00 | 40.06 |
| ATOM | 3153 | OH2 | TIP3 | 160 | 6.414 | 3.927 | 16.889 | 1.00 | 37.07 |
| ATOM | 3156 | OH2 | TIP3 | 161 | -10.282 | 6.603 | 4.715 | 1.00 | 38.48 |
| ATOM | 3159 | OH2 | TIP3 | 162 | 76.410 | 1.681 | -0.781 | 1.00 | 42.87 |
| ATOM | 3162 | OH2 | TIP3 | 163 | 9.910 | -12.046 | 17.157 | 1.00 | 32.79 |
| ATOM | 3165 | OH2 | TIP3 | 164 | 33.983 | 14.219 | 18.191 | 1.00 | 37.35 |
| ATOM | 3168 | OH2 | TIP3 | 165 | 2.330 | -7.952 | 16.978 | 1.00 | 44.25 |
| ATOM | 3171 | OH2 | TIP3 | 166 | 29.701 | 1.780 | 5.987 | 1.00 | 39.86 |
| ATOM | 3174 | OH2 | TIP3 | 167 | 32.494 | -17.319 | 11.798 | 1.00 | 38.46 |
| ATOM | 3177 | OH2 | TIP3 | 168 | 42.107 | 17.932 | 10.978 | 1.00 | 44.83 |
| ATOM | 3180 | OH2 | TIP3 | 169 | 87.822 | 10.537 | 5.568 | 1.00 | 54.30 |
| ATOM | 3183 | OH2 | TIP3 | 170 | 70.261 | -4.143 | 25.064 | 1.00 | 44.75 |
| ATOM | 3186 | OH2 | TIP3 | 171 | 77.519 | 5.882 | 23.891 | 1.00 | 42.67 |
| ATOM | 3189 | OH2 | TIP3 | 172 | -0.921 | -8.166 | 4.521 | 1.00 | 45.91 |
| ATOM | 3192 | OH2 | TIP3 | 173 | 34.213 | 15.329 | 1.478 | 1.00 | 40.10 |
| ATOM | 3195 | OH2 | TIP3 | 174 | -9.647 | 7.731 | 7.383 | 1.00 | 35.63 |
| ATOM | 3198 | OH2 | TIP3 | 175 | 11.619 | 5.799 | 7.440 | 1.00 | 36.36 |
| ATOM | 3201 | OH2 | TIP3 | 176 | -8.709 | 13.964 | 13.507 | 1.00 | 51.97 |
| ATOM | 3204 | OH2 | TIP3 | 177 | 31.770 | 3.376 | 18.354 | 1.00 | 46.26 |
| ATOM | 3207 | OH2 | TIP3 | 178 | -8.494 | 9.789 | 24.269 | 1.00 | 50.98 |
| ATOM | 3210 | OH2 | TIP3 | 179 | -1.234 | -6.253 | 15.622 | 1.00 | 38.47 |
| ATOM | 3213 | OH2 | TIP3 | 180 | 80.252 | 0.887 | 15.691 | 1.00 | 39.48 |
| ATOM | 3216 | OH2 | TIP3 | 181 | 67.248 | 20.272 | -1.555 | 1.00 | 48.22 |
| ATOM | 3219 | OH2 | TIP3 | 182 | -0.566 | 4.367 | 1.362 | 1.00 | 39.84 |
| ATOM | 3222 | OH2 | TIP3 | 183 | 0.120 | 6.523 | 2.615 | 1.00 | 33.11 |
| ATOM | 3225 | OH2 | TIP3 | 184 | -1.496 | 8.789 | 1.237 | 1.00 | 41.03 |
| ATOM | 3228 | OH2 | TIP3 | 185 | -5.143 | 9.130 | 2.236 | 1.00 | 40.47 |
| ATOM | 3231 | OH2 | TIP3 | 186 | -7.275 | 10.106 | 3.833 | 1.00 | 40.55 |
| ATOM | 3234 | OH2 | TIP3 | 187 | 2.717 | 7.275 | 0.769 | 1.00 | 44.67 |
| ATOM | 3237 | OH2 | TIP3 | 188 | 5.176 | 10.645 | 8.459 | 1.00 | 34.48 |
| ATOM | 3240 | OH2 | TIP3 | 189 | 63.822 | 12.690 | 22.883 | 1.00 | 41.88 |
| ATOM | 3243 | OH2 | TIP3 | 190 | 79.109 | 1.028 | 18.201 | 1.00 | 46.40 |
| ATOM | 3246 | OH2 | TIP3 | 191 | 59.332 | -11.681 | 7.236 | 1.00 | 63.45 |
| ATOM | 3249 | OH2 | TIP3 | 192 | 13.967 | -1.218 | -4.268 | 1.00 | 34.79 |
| ATOM | 3252 | OH2 | TIP3 | 193 | 59.444 | 2.867 | 33.368 | 1.00 | 41.00 |
| ATOM | 3255 | OH2 | TIP3 | 194 | 32.024 | 13.487 | 19.852 | 1.00 | 53.61 |
| ATOM | 3258 | OH2 | TIP3 | 195 | 72.101 | 16.218 | 22.802 | 1.00 | 44.03 |
| ATOM | 3261 | OH2 | TIP3 | 196 | 0.987 | -8.546 | 14.474 | 1.00 | 41.38 |
| ATOM | 3264 | OH2 | TIP3 | 197 | -0.491 | 5.461 | 30.372 | 1.00 | 38.51 |
| ATOM | 3267 | OH2 | TIP3 | 198 | 61.179 | 6.795 | 11.905 | 1.00 | 41.77 |
| ATOM | 3270 | OH2 | TIP3 | 199 | -1.365 | -4.128 | 27.656 | 1.00 | 50.98 |
| ATOM | 3273 | OH2 | TIP3 | 200 | 81.440 | 15.558 | 17.262 | 1.00 | 44.47 |
| ATOM | 3276 | OH2 | TIP3 | 201 | -17.491 | 4.116 | 23.873 | 1.00 | 50.58 |
| ATOM | 3279 | OH2 | TIP3 | 202 | 27.546 | 10.513 | 14.499 | 1.00 | 39.06 |
| ATOM | 3282 | OH2 | TIP3 | 203 | 34.992 | 4.513 | 27.719 | 1.00 | 49.89 |
| ATOM | 3285 | OH2 | TIP3 | 204 | -3.486 | -4.591 | 9.171 | 1.00 | 49.53 |
| ATOM | 3288 | OH2 | TIP3 | 205 | 42.799 | 7.848 | 22.320 | 1.00 | 43.50 |

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ATOM   3291  OH2   TIP3  206     52.728    11.884   21.811   1.00   39.98
ATOM   3294  OH2   TIP3  207     26.706    14.069   19.833   1.00   46.68
ATOM   3297  OH2   TIP3  208     -7.154     8.907    6.444   1.00   42.83
ATOM   3300  OH2   TIP3  209     86.648     5.606   16.034   1.00   51.15
ATOM   3303  OH2   TIP3  210     54.879    15.840   20.379   1.00   50.23
ATOM   3306  OH2   TIP3  211     51.417    19.473   22.691   1.00   48.35
ATOM   3309  OH2   TIP3  212     20.102     6.924    7.085   1.00   38.15
ATOM   3312  OH2   TIP3  213     28.991     1.941   -3.570   1.00   47.39
ATOM   3315  OH2   TIP3  214     26.505     2.386   -4.633   1.00   46.48
ATOM   3318  OH2   TIP3  215     36.482     2.810   18.521   1.00   46.26
ATOM   3321  OH2   TIP3  216     16.941   -20.504   14.128   1.00   49.74
ATOM   3324  OH2   TIP3  217     28.572   -14.448    6.157   1.00   49.13
ATOM   3327  OH2   TIP3  218     31.380     1.471   -1.998   1.00   43.02
ATOM   3330  OH2   TIP3  219     10.065   -16.338   15.455   1.00   42.75
ATOM   3333  OH2   TIP3  220      7.350   -11.974    5.652   1.00   55.35
ATOM   3336  OH2   TIP3  221    -12.328    14.547   10.986   1.00   51.29
ATOM   3339  OH2   TIP3  222     11.186     9.609   -1.388   1.00   37.68
ATOM   3342  OH2   TIP3  223     11.389    12.276   -1.400   1.00   46.93
ATOM   3345  OH2   TIP3  224     34.202    13.069   -1.161   1.00   41.79
ATOM   3348  OH2   TIP3  225     31.303    17.822    7.853   1.00   48.21
ATOM   3351  OH2   TIP3  226     36.875    11.804   -2.106   1.00   59.03
ATOM   3354  OH2   TIP3  227     35.134     3.048   11.020   1.00   50.41
ATOM   3357  OH2   TIP3  228     63.950    13.409   26.627   1.00   43.40
ATOM   3360  OH2   TIP3  229     36.367     6.116   15.221   1.00   57.79
ATOM   3363  OH2   TIP3  230     90.606     4.355    6.342   1.00   47.53
ATOM   3366  OH2   TIP3  231     50.038   -11.673   10.767   1.00   56.90
ATOM   3369  OH2   TIP3  232     60.196   -10.144   16.590   1.00   51.61
ATOM   3372  OH2   TIP3  233     18.021   -21.179    7.008   1.00   49.93
ATOM   3375  OH2   TIP3  234     66.236    -1.218   30.583   1.00   39.55
ATOM   3378  OH2   TIP3  235     74.959    18.928   20.659   1.00   38.04
ATOM   3381  OH2   TIP3  236     -2.816    10.082    3.187   1.00   49.31
ATOM   3384  OH2   TIP3  237      5.894    -3.410   25.289   1.00   35.55
ATOM   3387  OH2   TIP3  238     35.784     6.047   12.543   1.00   41.96
ATOM   3390  OH2   TIP3  239     -5.400    16.537   14.180   1.00   43.13
ATOM   3393  OH2   TIP3  240     46.589   -11.622   26.970   1.00   43.71
ATOM   3396  OH2   TIP3  241      6.199     6.592   13.797   1.00   46.51
ATOM   3399  OH2   TIP3  242     -3.777    -5.158   20.907   1.00   42.08
ATOM   3402  OH2   TIP3  243      1.969    -3.711   -0.282   1.00   37.38
ATOM   3405  OH2   TIP3  244     86.200    11.629   22.877   1.00   56.51
ATOM   3408  OH2   TIP3  245     10.557     7.565    5.514   1.00   47.58
ATOM   3411  OH2   TIP3  246      4.802     8.149    2.136   1.00   50.70
ATOM   3414  OH2   TIP3  247     64.590    -8.128   20.596   1.00   43.65
ATOM   3417  OH2   TIP3  248     11.346   -17.840   13.283   1.00   47.64
ATOM   3420  OH2   TIP3  249     42.116    -6.808   14.953   1.00   53.79
ATOM   3423  OH2   TIP3  250      2.745    -4.054   22.128   1.00   60.88
ATOM   3426  OH2   TIP3  251     71.999     1.177   -2.124   1.00   47.90
ATOM   3429  OH2   TIP3  252     50.328    -3.210   33.068   1.00   57.01
ATOM   3435  OH2   TIP3  253     57.838     9.337   11.631   1.00   52.55
ATOM   3438  OH2   TIP3  254     43.373    20.489   30.490   1.00   51.97
ATOM   3441  OH2   TIP3  255     67.045    16.529   15.793   1.00   49.02
ATOM   3444  OH2   TIP3  256     87.509    21.566    5.114   1.00   54.21
ATOM   3447  OH2   TIP3  257     21.060    10.052   -9.215   1.00   60.32
ATOM   3450  OH2   TIP3  258     11.827     2.450   27.951   1.00   54.26
ATOM   3453  OH2   TIP3  259     64.788    -0.418    3.563   1.00   50.94
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3456 | OH2 | TIP3 | 260 | 71.859 | 28.473 | 7.950 | 1.00 | 62.81 |
| ATOM | 3459 | OH2 | TIP3 | 261 | 25.605 | -8.106 | 27.287 | 1.00 | 52.81 |
| ATOM | 3462 | OH2 | TIP3 | 262 | -18.804 | 10.886 | 12.628 | 1.00 | 55.25 |
| ATOM | 3465 | OH2 | TIP3 | 263 | 30.652 | 11.349 | 16.201 | 1.00 | 50.40 |
| ATOM | 3468 | OH2 | TIP3 | 264 | 22.350 | -16.098 | -2.742 | 1.00 | 53.27 |
| ATOM | 3471 | OH2 | TIP3 | 265 | 29.720 | 9.106 | 18.465 | 1.00 | 57.23 |

## TABLE 2

| Atom No. | | Atom Type | A.A Type | A.A No. | X | Y | Z | OCC | B |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1 | N | GLU | 1464 | -13.425 | 16.769 | 8.973 | 1.00 | 61.21 |
| ATOM | 3 | CA | GLU | 1464 | -12.536 | 16.852 | 7.821 | 1.00 | 59.70 |
| ATOM | 4 | CB | GLU | 1464 | -11.383 | 17.829 | 8.085 | 1.00 | 60.05 |
| ATOM | 5 | C | GLU | 1464 | -11.998 | 15.478 | 7.427 | 1.00 | 57.11 |
| ATOM | 6 | O | GLU | 1464 | -12.134 | 15.076 | 6.274 | 1.00 | 59.75 |
| ATOM | 7 | N | LEU | 1465 | -11.406 | 14.749 | 8.368 | 1.00 | 52.21 |
| ATOM | 9 | CA | LEU | 1465 | -10.871 | 13.424 | 8.062 | 1.00 | 46.72 |
| ATOM | 10 | CB | LEU | 1465 | -10.102 | 12.844 | 9.249 | 1.00 | 44.98 |
| ATOM | 11 | CG | LEU | 1465 | -8.608 | 13.123 | 9.384 | 1.00 | 46.11 |
| ATOM | 12 | CD1 | LEU | 1465 | -8.338 | 14.592 | 9.663 | 1.00 | 51.13 |
| ATOM | 13 | CD2 | LEU | 1465 | -8.064 | 12.286 | 10.512 | 1.00 | 4.99 |
| ATOM | 14 | C | LEU | 1465 | -12.000 | 12.475 | 7.700 | 1.00 | 44.16 |
| ATOM | 15 | O | LEU | 1465 | -13.101 | 12.577 | 8.239 | 1.00 | 44.04 |
| ATOM | 16 | N | PRO | 1466 | -11.760 | 11.580 | 6.732 | 1.00 | 42.53 |
| ATOM | 17 | CD | PRO | 1466 | -10.535 | 11.534 | 5.913 | 1.00 | 41.30 |
| ATOM | 18 | CA | PRO | 1466 | -12.740 | 10.591 | 6.269 | 1.00 | 41.16 |
| ATOM | 19 | CB | PRO | 1466 | -12.134 | 10.111 | 4.959 | 1.00 | 41.48 |
| ATOM | 20 | CG | PRO | 1466 | -10.658 | 10.213 | 5.220 | 1.00 | 41.30 |
| ATOM | 21 | C | PRO | 1466 | -12.906 | 9.441 | 7.261 | 1.00 | 41.31 |
| ATOM | 22 | O | PRO | 1466 | -11.929 | 8.936 | 7.816 | 1.00 | 41.05 |
| ATOM | 23 | N | GLU | 1467 | -14.145 | 9.044 | 7.500 | 1.00 | 41.02 |
| ATOM | 25 | CA | GLU | 1467 | -14.428 | 7.960 | 8.427 | 1.00 | 42.42 |
| ATOM | 26 | CB | GLU | 1467 | -15.931 | 7.904 | 8.712 | 1.00 | 47.98 |
| ATOM | 27 | CG | GLU | 1467 | -16.565 | 9.238 | 9.105 | 1.00 | 52.79 |
| ATOM | 28 | CD | GLU | 1467 | -17.998 | 9.093 | 9.606 | 1.00 | 54.21 |
| ATOM | 29 | OE1 | GLU | 1467 | -18.474 | 7.949 | 9.741 | 1.00 | 58.90 |
| ATOM | 30 | OE2 | GLU | 1467 | -18.650 | 10.120 | 9.879 | 1.00 | 55.90 |
| ATOM | 31 | C | GLU | 1467 | -13.972 | 6.628 | 7.837 | 1.00 | 40.93 |
| ATOM | 32 | O | GLU | 1467 | -14.061 | 6.426 | 6.620 | 1.00 | 44.32 |
| ATOM | 33 | N | ASP | 1468 | -13.473 | 5.731 | 8.689 | 1.00 | 35.10 |
| ATOM | 35 | CA | ASP | 1468 | -13.024 | 4.404 | 8.256 | 1.00 | 31.82 |
| ATOM | 36 | CB | ASP | 1468 | -11.507 | 4.358 | 7.992 | 1.00 | 30.65 |
| ATOM | 37 | CG | ASP | 1468 | -11.025 | 3.002 | 7.440 | 1.00 | 29.93 |
| ATOM | 38 | OD1 | ASP | 1468 | -11.689 | 1.958 | 7.603 | 1.00 | 29.63 |
| ATOM | 39 | OD2 | ASP | 1468 | -9.945 | 2.974 | 6.835 | 1.00 | 33.63 |
| ATOM | 40 | C | ASP | 1468 | -13.394 | 3.441 | 9.369 | 1.00 | 31.81 |
| ATOM | 41 | O | ASP | 1468 | -12.618 | 3.209 | 10.302 | 1.00 | 31.91 |
| ATOM | 42 | N | PRO | 1469 | -14.569 | 2.819 | 9.247 | 1.00 | 29.68 |
| ATOM | 43 | CD | PRO | 1469 | -15.482 | 2.963 | 8.097 | 1.00 | 28.33 |
| ATOM | 44 | CA | PRO | 1469 | -15.100 | 1.863 | 10.220 | 1.00 | 31.80 |
| ATOM | 45 | CB | PRO | 1469 | -16.352 | 1.331 | 9.510 | 1.00 | 32.51 |
| ATOM | 46 | CG | PRO | 1469 | -16.783 | 2.496 | 8.656 | 1.00 | 27.41 |
| ATOM | 47 | C | PRO | 1469 | -14.146 | 0.731 | 10.590 | 1.00 | 30.44 |
| ATOM | 48 | O | PRO | 1469 | -14.272 | 0.135 | 11.654 | 1.00 | 30.02 |
| ATOM | 49 | N | ARG | 1470 | -13.198 | 0.442 | 9.704 | 1.00 | 31.06 |
| ATOM | 51 | CA | ARG | 1470 | -12.240 | -0.636 | 9.917 | 1.00 | 31.86 |
| ATOM | 52 | CB | ARG | 1470 | -11.386 | -0.860 | 8.660 | 1.00 | 31.36 |
| ATOM | 53 | CG | ARG | 1470 | -12.107 | -1.437 | 7.448 | 1.00 | 33.08 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 54 | CD | ARG | 1470 | -11.148 | -1.588 | 6.248 | 1.00 | 31.08 |
| ATOM | 55 | NE | ARG | 1470 | -10.540 | -0.310 | 5.891 | 1.00 | 34.36 |
| ATOM | 57 | CZ | ARG | 1470 | -9.656 | -0.135 | 4.919 | 1.00 | 33.32 |
| ATOM | 58 | NH1 | ARG | 1470 | -9.260 | -1.164 | 4.185 | 1.00 | 35.90 |
| ATOM | 61 | NH2 | ARG | 1470 | -9.155 | 1.074 | 4.687 | 1.00 | 32.79 |
| ATOM | 64 | C | ARG | 1470 | -11.290 | -0.436 | 11.095 | 1.00 | 32.68 |
| ATOM | 65 | O | ARG | 1470 | -10.820 | -1.410 | 11.683 | 1.00 | 33.43 |
| ATOM | 66 | N | TRP | 1471 | -11.031 | 0.814 | 11.456 | 1.00 | 31.84 |
| ATOM | 68 | CA | TRP | 1471 | -10.063 | 1.090 | 12.505 | 1.00 | 31.17 |
| ATOM | 69 | CB | TRP | 1471 | -8.816 | 1.677 | 11.850 | 1.00 | 30.15 |
| ATOM | 70 | CG | TRP | 1471 | -8.173 | 0.725 | 10.941 | 1.00 | 29.54 |
| ATOM | 71 | CD2 | TRP | 1471 | -7.288 | -0.329 | 11.315 | 1.00 | 31.07 |
| ATOM | 72 | CE2 | TRP | 1471 | -6.913 | -0.992 | 10.132 | 1.00 | 34.41 |
| ATOM | 73 | CE3 | TRP | 1471 | -6.762 | -0.768 | 12.536 | 1.00 | 29.46 |
| ATOM | 74 | CD1 | TRP | 1471 | -8.309 | 0.660 | 9.587 | 1.00 | 30.20 |
| ATOM | 75 | NE1 | TRP | 1471 | -7.557 | -0.371 | 9.089 | 1.00 | 33.09 |
| ATOM | 77 | CZ2 | TRP | 1471 | -6.042 | -2.085 | 10.135 | 1.00 | 31.68 |
| ATOM | 78 | CZ3 | TRP | 1471 | -5.897 | -1.853 | 12.540 | 1.00 | 29.65 |
| ATOM | 79 | CH2 | TRP | 1471 | -5.541 | -2.494 | 11.347 | 1.00 | 30.18 |
| ATOM | 80 | C | TRP | 1471 | -10.477 | 2.019 | 13.620 | 1.00 | 29.94 |
| ATOM | 81 | O | TRP | 1471 | -9.782 | 2.108 | 14.631 | 1.00 | 30.00 |
| ATOM | 82 | N | GLU | 1472 | -11.573 | 2.737 | 13.416 | 1.00 | 29.06 |
| ATOM | 84 | CA | GLU | 1472 | -12.051 | 3.706 | 14.380 | 1.00 | 28.62 |
| ATOM | 85 | CB | GLU | 1472 | -13.312 | 4.386 | 13.849 | 1.00 | 29.16 |
| ATOM | 86 | CG | GLU | 1472 | -13.641 | 5.733 | 14.529 | 1.00 | 30.74 |
| ATOM | 87 | CD | GLU | 1472 | -12.676 | 6.848 | 14.156 | 1.00 | 30.05 |
| ATOM | 88 | OE1 | GLU | 1472 | -12.090 | 6.799 | 13.057 | 1.00 | 31.32 |
| ATOM | 89 | OE2 | GLU | 1472 | -12.511 | 7.784 | 14.961 | 1.00 | 30.26 |
| ATOM | 90 | C | GLU | 1472 | -12.327 | 3.159 | 15.767 | 1.00 | 28.70 |
| ATOM | 91 | O | GLU | 1472 | -12.969 | 2.125 | 15.916 | 1.00 | 31.01 |
| ATOM | 92 | N | LEU | 1473 | -11.810 | 3.842 | 16.781 | 1.00 | 27.38 |
| ATOM | 94 | CA | LEU | 1473 | -12.054 | 3.451 | 18.161 | 1.00 | 29.61 |
| ATOM | 95 | CB | LEU | 1473 | -10.763 | 3.073 | 18.899 | 1.00 | 28.56 |
| ATOM | 96 | CG | LEU | 1473 | -10.923 | 2.756 | 20.403 | 1.00 | 30.06 |
| ATOM | 97 | CD1 | LEU | 1473 | -11.485 | 1.354 | 20.639 | 1.00 | 28.42 |
| ATOM | 98 | CD2 | LEU | 1473 | -9.595 | 2.876 | 21.115 | 1.00 | 28.15 |
| ATOM | 99 | C | LEU | 1473 | -12.617 | 4.714 | 18.764 | 1.00 | 31.81 |
| ATOM | 100 | O | LEU | 1473 | -12.179 | 5.814 | 18.407 | 1.00 | 33.00 |
| ATOM | 101 | N | PRO | 1474 | -13.670 | 4.591 | 19.596 | 1.00 | 31.45 |
| ATOM | 102 | CD | PRO | 1474 | -14.488 | 3.400 | 19.859 | 1.00 | 31.72 |
| ATOM | 103 | CA | PRO | 1474 | -14.261 | 5.774 | 20.226 | 1.00 | 31.23 |
| ATOM | 104 | CB | PRO | 1474 | -15.400 | 5.176 | 21.048 | 1.00 | 29.01 |
| ATOM | 105 | CG | PRO | 1474 | -15.815 | 4.005 | 20.247 | 1.00 | 29.09 |
| ATOM | 106 | C | PRO | 1474 | -13.217 | 6.444 | 21.120 | 1.00 | 33.36 |
| ATOM | 107 | O | PRO | 1474 | -12.447 | 5.765 | 21.808 | 1.00 | 36.40 |
| ATOM | 108 | N | ARG | 1475 | -13.188 | 7.770 | 21.112 | 1.00 | 33.67 |
| ATOM | 110 | CA | ARG | 1475 | -12.228 | 8.498 | 21.924 | 1.00 | 33.96 |
| ATOM | 111 | CB | ARG | 1475 | -12.433 | 9.991 | 21.735 | 1.00 | 35.31 |
| ATOM | 112 | CG | ARG | 1475 | -12.134 | 10.405 | 20.333 | 1.00 | 40.10 |
| ATOM | 113 | CD | ARG | 1475 | -12.060 | 11.906 | 20.145 | 1.00 | 42.98 |
| ATOM | 114 | NE | ARG | 1475 | -11.785 | 12.194 | 18.737 | 1.00 | 42.91 |
| ATOM | 116 | CZ | ARG | 1475 | -10.578 | 12.443 | 18.253 | 1.00 | 41.30 |
| ATOM | 117 | NH1 | ARG | 1475 | -9.529 | 12.467 | 19.064 | 1.00 | 41.88 |
| ATOM | 120 | NH2 | ARG | 1475 | -10.413 | 12.567 | 16.943 | 1.00 | 40.98 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 123 | C | ARG | 1475 | -12.278 | 8.142 | 23.404 | 1.00 | 35.88 |
| ATOM | 124 | O | ARG | 1475 | -11.240 | 8.046 | 24.061 | 1.00 | 37.10 |
| ATOM | 125 | N | ASP | 1476 | -13.479 | 7.920 | 23.928 | 1.00 | 36.47 |
| ATOM | 127 | CA | ASP | 1476 | -13.632 | 7.581 | 25.335 | 1.00 | 37.24 |
| ATOM | 128 | CB | ASP | 1476 | -15.112 | 7.629 | 25.741 | 1.00 | 39.66 |
| ATOM | 129 | CG | ASP | 1476 | -15.930 | 6.480 | 25.163 | 1.00 | 42.38 |
| ATOM | 130 | OD1 | ASP | 1476 | -15.438 | 5.706 | 24.322 | 1.00 | 47.52 |
| ATOM | 131 | OD2 | ASP | 1476 | -17.098 | 6.349 | 25.568 | 1.00 | 48.06 |
| ATOM | 132 | C | ASP | 1476 | -13.023 | 6.232 | 25.724 | 1.00 | 36.93 |
| ATOM | 133 | O | ASP | 1476 | -13.034 | 5.856 | 26.898 | 1.00 | 40.09 |
| ATOM | 134 | N | ARG | 1477 | -12.564 | 5.475 | 24.732 | 1.00 | 34.34 |
| ATOM | 136 | CA | ARG | 1477 | -11.961 | 4.171 | 24.993 | 1.00 | 32.47 |
| ATOM | 137 | CB | ARG | 1477 | -12.269 | 3.212 | 23.852 | 1.00 | 31.59 |
| ATOM | 138 | CG | ARG | 1477 | -13.716 | 2.939 | 23.640 | 1.00 | 29.66 |
| ATOM | 139 | CD | ARG | 1477 | -14.314 | 2.342 | 24.875 | 1.00 | 30.65 |
| ATOM | 140 | NE | ARG | 1477 | -14.498 | 3.342 | 25.918 | 1.00 | 31.37 |
| ATOM | 142 | CZ | ARG | 1477 | -14.822 | 3.055 | 27.174 | 1.00 | 32.81 |
| ATOM | 143 | NH1 | ARG | 1477 | -15.002 | 1.794 | 27.549 | 1.00 | 33.92 |
| ATOM | 146 | NH2 | ARG | 1477 | -14.950 | 4.025 | 28.062 | 1.00 | 31.74 |
| ATOM | 149 | C | ARG | 1477 | -10.452 | 4.266 | 25.153 | 1.00 | 33.13 |
| ATOM | 150 | O | ARG | 1477 | -9.777 | 3.281 | 25.445 | 1.00 | 33.55 |
| ATOM | 151 | N | LEU | 1478 | -9.923 | 5.466 | 24.984 | 1.00 | 34.43 |
| ATOM | 153 | CA | LEU | 1478 | -8.493 | 5.663 | 25.076 | 1.00 | 35.68 |
| ATOM | 154 | CB | LEU | 1478 | -8.008 | 6.350 | 23.790 | 1.00 | 34.98 |
| ATOM | 155 | CG | LEU | 1478 | -6.581 | 6.137 | 23.284 | 1.00 | 31.11 |
| ATOM | 156 | CD1 | LEU | 1478 | -6.280 | 4.650 | 23.161 | 1.00 | 26.62 |
| ATOM | 157 | CD2 | LEU | 1478 | -6.428 | 6.839 | 21.940 | 1.00 | 28.80 |
| ATOM | 158 | C | LEU | 1478 | -8.158 | 6.505 | 26.295 | 1.00 | 36.21 |
| ATOM | 159 | O | LEU | 1478 | -8.501 | 7.688 | 26.361 | 1.00 | 39.67 |
| ATOM | 160 | N | VAL | 1479 | -7.558 | 5.878 | 27.293 | 1.00 | 35.42 |
| ATOM | 162 | CA | VAL | 1479 | -7.156 | 6.599 | 28.491 | 1.00 | 35.80 |
| ATOM | 163 | CB | VAL | 1479 | -7.269 | 5.707 | 29.742 | 1.00 | 36.29 |
| ATOM | 164 | CG1 | VAL | 1479 | -7.017 | 6.527 | 30.983 | 1.00 | 37.23 |
| ATOM | 165 | CG2 | VAL | 1479 | -8.650 | 5.059 | 29.812 | 1.00 | 34.41 |
| ATOM | 166 | C | VAL | 1479 | -5.704 | 7.046 | 28.244 | 1.00 | 35.68 |
| ATOM | 167 | O | VAL | 1479 | -4.764 | 6.246 | 28.319 | 1.00 | 33.45 |
| ATOM | 168 | N | LEU | 1480 | -5.538 | 8.315 | 27.885 | 1.00 | 38.15 |
| ATOM | 170 | CA | LEU | 1480 | -4.213 | 8.860 | 27.584 | 1.00 | 42.61 |
| ATOM | 171 | CB | LEU | 1480 | -4.332 | 10.205 | 26.857 | 1.00 | 39.14 |
| ATOM | 172 | CG | LEU | 1480 | -4.969 | 10.179 | 25.460 | 1.00 | 38.44 |
| ATOM | 173 | CD1 | LEU | 1480 | -4.901 | 11.579 | 24.879 | 1.00 | 39.39 |
| ATOM | 174 | CD2 | LEU | 1480 | -4.263 | 9.194 | 24.533 | 1.00 | 36.86 |
| ATOM | 175 | C | LEU | 1480 | -3.274 | 8.970 | 28.783 | 1.00 | 46.37 |
| ATOM | 176 | O | LEU | 1480 | -3.659 | 9.445 | 29.850 | 1.00 | 48.86 |
| ATOM | 177 | N | GLY | 1481 | -2.033 | 8.537 | 28.594 | 1.00 | 47.13 |
| ATOM | 179 | CA | GLY | 1481 | -1.081 | 8.573 | 29.678 | 1.00 | 48.19 |
| ATOM | 180 | C | GLY | 1481 | 0.163 | 9.388 | 29.425 | 1.00 | 50.27 |
| ATOM | 181 | O | GLY | 1481 | 0.152 | 10.367 | 28.675 | 1.00 | 51.19 |
| ATOM | 182 | N | LYS | 1482 | 1.240 | 8.965 | 30.078 | 1.00 | 50.93 |
| ATOM | 184 | CA | LYS | 1482 | 2.543 | 9.606 | 30.007 | 1.00 | 50.94 |
| ATOM | 185 | CB | LYS | 1482 | 3.509 | 8.866 | 30.933 | 1.00 | 50.41 |
| ATOM | 186 | CG | LYS | 1482 | 4.971 | 9.026 | 30.567 | 1.00 | 51.87 |
| ATOM | 187 | CD | LYS | 1482 | 5.810 | 7.874 | 31.087 | 1.00 | 53.49 |
| ATOM | 188 | CE | LYS | 1482 | 5.390 | 6.542 | 30.478 | 1.00 | 50.77 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 189 | NZ | LYS | 1482 | 6.251 | 5.433 | 30.986 | 1.00 | 49.92 |
| ATOM | 193 | C | LYS | 1482 | 3.145 | 9.676 | 28.609 | 1.00 | 52.31 |
| ATOM | 194 | O | LYS | 1482 | 3.115 | 8.700 | 27.851 | 1.00 | 52.30 |
| ATOM | 195 | N | PRO | 1483 | 3.706 | 10.838 | 28.250 | 1.00 | 53.47 |
| ATOM | 196 | CD | PRO | 1483 | 3.667 | 12.105 | 28.997 | 1.00 | 54.19 |
| ATOM | 197 | CA | PRO | 1483 | 4.326 | 11.021 | 26.937 | 1.00 | 54.10 |
| ATOM | 198 | CB | PRO | 1483 | 4.772 | 12.480 | 26.976 | 1.00 | 54.25 |
| ATOM | 199 | CG | PRO | 1483 | 3.772 | 13.118 | 27.895 | 1.00 | 55.30 |
| ATOM | 200 | C | PRO | 1483 | 5.535 | 10.096 | 26.827 | 1.00 | 54.72 |
| ATOM | 201 | O | PRO | 1483 | 6.343 | 10.017 | 27.751 | 1.00 | 53.48 |
| ATOM | 202 | N | LEU | 1484 | 5.619 | 9.351 | 25.731 | 1.00 | 57.05 |
| ATOM | 204 | CA | LEU | 1484 | 6.739 | 8.447 | 25.503 | 1.00 | 59.26 |
| ATOM | 205 | CB | LEU | 1484 | 6.307 | 7.241 | 24.669 | 1.00 | 59.35 |
| ATOM | 206 | CG | LEU | 1484 | 5.391 | 6.216 | 25.343 | 1.00 | 60.87 |
| ATOM | 207 | CD1 | LEU | 1484 | 4.975 | 5.161 | 24.329 | 1.00 | 57.14 |
| ATOM | 208 | CD2 | LEU | 1484 | 6.081 | 5.571 | 26.551 | 1.00 | 59.79 |
| ATOM | 209 | C | LEU | 1484 | 7.847 | 9.194 | 24.778 | 1.00 | 61.30 |
| ATOM | 210 | O | LEU | 1484 | 8.980 | 8.720 | 24.701 | 1.00 | 62.17 |
| ATOM | 211 | N | GLY | 1485 | 7.494 | 10.351 | 24.220 | 1.00 | 63.75 |
| ATOM | 213 | CA | GLY | 1485 | 8.456 | 11.173 | 23.507 | 1.00 | 66.33 |
| ATOM | 214 | C | GLY | 1485 | 8.081 | 11.412 | 22.054 | 1.00 | 67.79 |
| ATOM | 215 | O | GLY | 1485 | 6.918 | 11.653 | 21.727 | 1.00 | 69.61 |
| ATOM | 216 | N | GLN | 1491 | 4.615 | 13.762 | 18.385 | 1.00 | 58.26 |
| ATOM | 218 | CA | GLN | 1491 | 4.353 | 13.353 | 19.762 | 1.00 | 57.98 |
| ATOM | 219 | CB | GLN | 1491 | 3.476 | 14.379 | 20.468 | 1.00 | 61.80 |
| ATOM | 220 | CG | GLN | 1491 | 3.134 | 14.034 | 21.920 | 1.00 | 70.31 |
| ATOM | 221 | CD | GLN | 1491 | 2.019 | 14.911 | 22.482 | 1.00 | 75.91 |
| ATOM | 222 | OE1 | GLN | 1491 | 1.355 | 15.636 | 21.748 | 1.00 | 77.85 |
| ATOM | 223 | NE2 | GLN | 1491 | 1.820 | 14.832 | 23.788 | 1.00 | 78.30 |
| ATOM | 226 | C | GLN | 1491 | 3.709 | 11.965 | 19.881 | 1.00 | 54.67 |
| ATOM | 227 | O | GLN | 1491 | 2.701 | 11.669 | 19.222 | 1.00 | 54.91 |
| ATOM | 228 | N | VAL | 1492 | 4.305 | 11.125 | 20.729 | 1.00 | 50.04 |
| ATOM | 230 | CA | VAL | 1492 | 3.825 | 9.763 | 20.988 | 1.00 | 44.93 |
| ATOM | 231 | CB | VAL | 1492 | 4.861 | 8.705 | 20.583 | 1.00 | 42.65 |
| ATOM | 232 | CG1 | VAL | 1492 | 4.378 | 7.325 | 20.958 | 1.00 | 39.71 |
| ATOM | 233 | CG2 | VAL | 1492 | 5.119 | 8.766 | 19.099 | 1.00 | 40.98 |
| ATOM | 234 | C | VAL | 1492 | 3.584 | 9.661 | 22.490 | 1.00 | 43.43 |
| ATOM | 235 | O | VAL | 1492 | 4.451 | 10.029 | 23.289 | 1.00 | 43.43 |
| ATOM | 236 | N | VAL | 1493 | 2.400 | 9.212 | 22.888 | 1.00 | 41.13 |
| ATOM | 238 | CA | VAL | 1493 | 2.107 | 9.080 | 24.304 | 1.00 | 38.77 |
| ATOM | 239 | CB | VAL | 1493 | 1.052 | 10.133 | 24.782 | 1.00 | 36.35 |
| ATOM | 240 | CG1 | VAL | 1493 | 1.410 | 11.508 | 24.287 | 1.00 | 36.06 |
| ATOM | 241 | CG2 | VAL | 1493 | -0.329 | 9.755 | 24.339 | 1.00 | 37.64 |
| ATOM | 242 | C | VAL | 1493 | 1.589 | 7.693 | 24.619 | 1.00 | 37.77 |
| ATOM | 243 | O | VAL | 1493 | 0.948 | 7.058 | 23.783 | 1.00 | 38.88 |
| ATOM | 244 | N | LEU | 1494 | 1.949 | 7.187 | 25.790 | 1.00 | 36.24 |
| ATOM | 246 | CA | LEU | 1494 | 1.468 | 5.880 | 26.205 | 1.00 | 35.92 |
| ATOM | 247 | CB | LEU | 1494 | 2.252 | 5.383 | 27.429 | 1.00 | 35.41 |
| ATOM | 248 | CG | LEU | 1494 | 1.886 | 4.009 | 28.004 | 1.00 | 36.21 |
| ATOM | 249 | CD1 | LEU | 1494 | 1.927 | 2.931 | 26.924 | 1.00 | 33.60 |
| ATOM | 250 | CD2 | LEU | 1494 | 2.835 | 3.670 | 29.145 | 1.00 | 36.03 |
| ATOM | 251 | C | LEU | 1494 | -0.010 | 6.095 | 26.564 | 1.00 | 35.27 |
| ATOM | 252 | O | LEU | 1494 | -0.425 | 7.215 | 26.887 | 1.00 | 34.35 |
| ATOM | 253 | N | ALA | 1495 | -0.807 | 5.043 | 26.468 | 1.00 | 34.93 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 255 | CA | ALA | 1495 | -2.220 | 5.145 | 26.768 | 1.00 | 34.44 |
| ATOM | 256 | CB | ALA | 1495 | -2.955 | 5.794 | 25.616 | 1.00 | 35.29 |
| ATOM | 257 | C | ALA | 1495 | -2.781 | 3.770 | 27.018 | 1.00 | 34.59 |
| ATOM | 258 | O | ALA | 1495 | -2.128 | 2.766 | 26.748 | 1.00 | 35.52 |
| ATOM | 259 | N | GLU | 1496 | -3.996 | 3.723 | 27.536 | 1.00 | 36.64 |
| ATOM | 261 | CA | GLU | 1496 | -4.652 | 2.462 | 27.806 | 1.00 | 37.57 |
| ATOM | 262 | CB | GLU | 1496 | -5.000 | 2.354 | 29.287 | 1.00 | 38.97 |
| ATOM | 263 | CG | GLU | 1496 | -3.769 | 2.304 | 30.185 | 1.00 | 41.79 |
| ATOM | 264 | CD | GLU | 1496 | -4.110 | 2.475 | 31.645 | 1.00 | 43.65 |
| ATOM | 265 | OE1 | GLU | 1496 | -4.408 | 3.617 | 32.036 | 1.00 | 42.97 |
| ATOM | 266 | OE2 | GLU | 1496 | -4.086 | 1.475 | 32.398 | 1.00 | 46.65 |
| ATOM | 267 | C | GLU | 1496 | -5.896 | 2.404 | 26.943 | 1.00 | 38.50 |
| ATOM | 268 | O | GLU | 1496 | -6.660 | 3.371 | 26.867 | 1.00 | 40.28 |
| ATOM | 269 | N | ALA | 1497 | -6.051 | 1.301 | 26.223 | 1.00 | 37.34 |
| ATOM | 271 | CA | ALA | 1497 | -7.194 | 1.131 | 25.352 | 1.00 | 37.42 |
| ATOM | 272 | CB | ALA | 1497 | -6.743 | 0.625 | 23.985 | 1.00 | 35.92 |
| ATOM | 273 | C | ALA | 1497 | -8.146 | 0.148 | 26.000 | 1.00 | 36.77 |
| ATOM | 274 | O | ALA | 1497 | -7.759 | -0.977 | 26.323 | 1.00 | 35.74 |
| ATOM | 275 | N | ILE | 1498 | -9.354 | 0.616 | 26.291 | 1.00 | 37.03 |
| ATOM | 277 | CA | ILE | 1498 | -10.378 | -0.224 | 26.896 | 1.00 | 36.80 |
| ATOM | 278 | CB | ILE | 1498 | -11.372 | 0.612 | 27.728 | 1.00 | 34.53 |
| ATOM | 279 | CG2 | ILE | 1498 | -12.373 | -0.290 | 28.425 | 1.00 | 34.59 |
| ATOM | 280 | CG1 | ILE | 1498 | -10.640 | 1.438 | 28.778 | 1.00 | 31.97 |
| ATOM | 281 | CD1 | ILE | 1498 | -11.552 | 2.344 | 29.541 | 1.00 | 31.12 |
| ATOM | 282 | C | ILE | 1498 | -11.126 | -0.807 | 25.709 | 1.00 | 38.72 |
| ATOM | 283 | O | ILE | 1498 | -11.647 | -0.066 | 24.879 | 1.00 | 37.74 |
| ATOM | 284 | N | GLY | 1499 | -11.137 | -2.126 | 25.590 | 1.00 | 40.98 |
| ATOM | 286 | CA | GLY | 1499 | -11.839 | -2.728 | 24.482 | 1.00 | 44.64 |
| ATOM | 287 | C | GLY | 1499 | -10.931 | -3.115 | 23.332 | 1.00 | 48.45 |
| ATOM | 288 | O | GLY | 1499 | -10.260 | -4.147 | 23.401 | 1.00 | 51.92 |
| ATOM | 289 | N | LEU | 1500 | -10.877 | -2.269 | 22.303 | 1.00 | 47.87 |
| ATOM | 291 | CA | LEU | 1500 | -10.076 | -2.530 | 21.102 | 1.00 | 46.80 |
| ATOM | 292 | CB | LEU | 1500 | -8.594 | -2.770 | 21.434 | 1.00 | 45.37 |
| ATOM | 293 | CG | LEU | 1500 | -7.543 | -1.661 | 21.293 | 1.00 | 44.84 |
| ATOM | 294 | CD1 | LEU | 1500 | -6.174 | -2.290 | 21.450 | 1.00 | 43.33 |
| ATOM | 295 | CD2 | LEU | 1500 | -7.623 | -0.959 | 19.948 | 1.00 | 40.43 |
| ATOM | 296 | C | LEU | 1500 | -10.631 | -3.737 | 20.349 | 1.00 | 45.63 |
| ATOM | 297 | O | LEU | 1500 | -10.797 | -4.823 | 20.915 | 1.00 | 44.42 |
| ATOM | 298 | N | PRO | 1505 | -13.569 | -5.910 | 25.549 | 1.00 | 52.13 |
| ATOM | 299 | CD | PRO | 1505 | -14.316 | -7.170 | 25.398 | 1.00 | 54.09 |
| ATOM | 300 | CA | PRO | 1505 | -14.451 | -4.828 | 25.999 | 1.00 | 50.46 |
| ATOM | 301 | CB | PRO | 1505 | -15.841 | -5.455 | 25.891 | 1.00 | 49.86 |
| ATOM | 302 | CG | PRO | 1505 | -15.586 | -6.898 | 26.193 | 1.00 | 52.17 |
| ATOM | 303 | C | PRO | 1505 | -14.136 | -4.370 | 27.422 | 1.00 | 47.75 |
| ATOM | 304 | O | PRO | 1505 | -14.148 | -3.180 | 27.710 | 1.00 | 47.93 |
| ATOM | 305 | N | ASN | 1506 | -13.778 | -5.313 | 28.285 | 1.00 | 46.20 |
| ATOM | 307 | CA | ASN | 1506 | -13.458 | -4.986 | 29.666 | 1.00 | 49.52 |
| ATOM | 308 | CB | ASN | 1506 | -14.310 | -5.829 | 30.612 | 1.00 | 52.42 |
| ATOM | 309 | CG | ASN | 1506 | -15.788 | -5.489 | 30.526 | 1.00 | 54.50 |
| ATOM | 310 | OD1 | ASN | 1506 | -16.179 | -4.331 | 30.680 | 1.00 | 57.16 |
| ATOM | 311 | ND2 | ASN | 1506 | -16.610 | -6.489 | 30.244 | 1.00 | 56.82 |
| ATOM | 314 | C | ASN | 1506 | -11.973 | -5.124 | 30.003 | 1.00 | 50.65 |
| ATOM | 315 | O | ASN | 1506 | -11.583 | -5.174 | 31.178 | 1.00 | 50.65 |
| ATOM | 316 | N | ARG | 1507 | -11.142 | -5.145 | 28.968 | 1.00 | 50.90 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 318 | CA | ARG | 1507 | -9.700 | -5.276 | 29.127 | 1.00 | 49.77 |
| ATOM | 319 | CB | ARG | 1507 | -9.192 | -6.483 | 28.339 | 1.00 | 55.81 |
| ATOM | 320 | CG | ARG | 1507 | -9.450 | -7.833 | 28.988 | 1.00 | 61.63 |
| ATOM | 321 | CD | ARG | 1507 | -8.408 | -8.149 | 30.041 | 1.00 | 66.01 |
| ATOM | 322 | NE | ARG | 1507 | -8.600 | -9.490 | 30.583 | 1.00 | 72.55 |
| ATOM | 324 | CZ | ARG | 1507 | -8.024 | -9.944 | 31.694 | 1.00 | 77.32 |
| ATOM | 325 | NH1 | ARG | 1507 | -7.198 | -9.169 | 32.392 | 1.00 | 78.41 |
| ATOM | 328 | NH2 | ARG | 1507 | -8.335 | -11.151 | 32.147 | 1.00 | 79.30 |
| ATOM | 331 | C | ARG | 1507 | -9.015 | -4.036 | 28.595 | 1.00 | 45.60 |
| ATOM | 332 | O | ARG | 1507 | -9.452 | -3.464 | 27.590 | 1.00 | 42.08 |
| ATOM | 333 | N | VAL | 1508 | -7.977 | -3.597 | 29.297 | 1.00 | 42.86 |
| ATOM | 335 | CA | VAL | 1508 | -7.216 | -2.443 | 28.858 | 1.00 | 40.75 |
| ATOM | 336 | CB | VAL | 1508 | -6.903 | -1.428 | 30.010 | 1.00 | 38.75 |
| ATOM | 337 | CG1 | VAL | 1508 | -8.184 | -1.015 | 30.702 | 1.00 | 43.29 |
| ATOM | 338 | CG2 | VAL | 1508 | -5.919 | -2.005 | 31.012 | 1.00 | 37.56 |
| ATOM | 339 | C | VAL | 1508 | -5.929 | -2.970 | 28.248 | 1.00 | 39.14 |
| ATOM | 340 | O | VAL | 1508 | -5.369 | -3.972 | 28.708 | 1.00 | 39.16 |
| ATOM | 341 | N | THR | 1509 | -5.517 | -2.345 | 27.157 | 1.00 | 37.26 |
| ATOM | 343 | CA | THR | 1509 | -4.298 | -2.737 | 26.486 | 1.00 | 36.52 |
| ATOM | 344 | CB | THR | 1509 | -4.571 | -3.187 | 25.019 | 1.00 | 37.83 |
| ATOM | 345 | OG1 | THR | 1509 | -5.423 | -4.340 | 25.011 | 1.00 | 43.88 |
| ATOM | 347 | CG2 | THR | 1509 | -3.267 | -3.540 | 24.310 | 1.00 | 34.51 |
| ATOM | 348 | C | THR | 1509 | -3.434 | -1.495 | 26.473 | 1.00 | 35.82 |
| ATOM | 349 | O | THR | 1509 | -3.927 | -0.408 | 26.174 | 1.00 | 34.37 |
| ATOM | 350 | N | LYS | 1510 | -2.175 | -1.628 | 26.880 | 1.00 | 35.96 |
| ATOM | 352 | CA | LYS | 1510 | -1.291 | -0.479 | 26.843 | 1.00 | 36.13 |
| ATOM | 353 | CB | LYS | 1510 | -0.032 | -0.695 | 27.680 | 1.00 | 37.77 |
| ATOM | 354 | CG | LYS | 1510 | -0.277 | -0.854 | 29.162 | 1.00 | 44.58 |
| ATOM | 355 | CD | LYS | 1510 | 1.023 | -0.658 | 29.948 | 1.00 | 51.33 |
| ATOM | 356 | CE | LYS | 1510 | 0.947 | -1.286 | 31.342 | 1.00 | 58.15 |
| ATOM | 357 | NZ | LYS | 1510 | -0.149 | -0.728 | 32.187 | 1.00 | 64.94 |
| ATOM | 361 | C | LYS | 1510 | -0.929 | -0.355 | 25.373 | 1.00 | 34.59 |
| ATOM | 362 | O | LYS | 1510 | -0.574 | -1.345 | 24.734 | 1.00 | 31.43 |
| ATOM | 363 | N | VAL | 1511 | -1.092 | 0.846 | 24.835 | 1.00 | 32.95 |
| ATOM | 365 | CA | VAL | 1511 | -0.810 | 1.121 | 23.441 | 1.00 | 32.29 |
| ATOM | 366 | CB | VAL | 1511 | -2.129 | 1.213 | 22.621 | 1.00 | 32.95 |
| ATOM | 367 | CG1 | VAL | 1511 | -2.879 | -0.109 | 22.686 | 1.00 | 34.79 |
| ATOM | 368 | CG2 | VAL | 1511 | -3.026 | 2.354 | 23.148 | 1.00 | 32.84 |
| ATOM | 369 | C | VAL | 1511 | -0.058 | 2.446 | 23.353 | 1.00 | 32.65 |
| ATOM | 370 | O | VAL | 1511 | 0.021 | 3.185 | 24.344 | 1.00 | 31.62 |
| ATOM | 371 | N | ALA | 1512 | 0.521 | 2.721 | 22.186 | 1.00 | 30.24 |
| ATOM | 373 | CA | ALA | 1512 | 1.244 | 3.969 | 21.954 | 1.00 | 28.18 |
| ATOM | 374 | CB | ALA | 1512 | 2.599 | 3.700 | 21.316 | 1.00 | 25.62 |
| ATOM | 375 | C | ALA | 1512 | 0.373 | 4.783 | 21.015 | 1.00 | 27.54 |
| ATOM | 376 | O | ALA | 1512 | -0.151 | 4.264 | 20.040 | 1.00 | 27.17 |
| ATOM | 377 | N | VAL | 1513 | 0.204 | 6.054 | 21.322 | 1.00 | 30.52 |
| ATOM | 379 | CA | VAL | 1513 | -0.630 | 6.914 | 20.503 | 1.00 | 34.08 |
| ATOM | 380 | CB | VAL | 1513 | -1.731 | 7.591 | 21.347 | 1.00 | 34.61 |
| ATOM | 381 | CG1 | VAL | 1513 | -2.607 | 8.444 | 20.474 | 1.00 | 36.75 |
| ATOM | 382 | CG2 | VAL | 1513 | -2.567 | 6.549 | 22.087 | 1.00 | 33.45 |
| ATOM | 383 | C | VAL | 1513 | 0.203 | 8.008 | 19.837 | 1.00 | 36.38 |
| ATOM | 384 | O | VAL | 1513 | 0.924 | 8.750 | 20.510 | 1.00 | 35.32 |
| ATOM | 385 | N | LYS | 1514 | 0.105 | 8.093 | 18.513 | 1.00 | 38.19 |
| ATOM | 387 | CA | LYS | 1514 | 0.818 | 9.104 | 17.746 | 1.00 | 40.12 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 388 | CB | LYS | 1514 | 1.339 | 8.513 | 16.439 | 1.00 | 40.93 |
| ATOM | 389 | CG | LYS | 1514 | 2.452 | 7.488 | 16.632 | 1.00 | 42.52 |
| ATOM | 390 | CD | LYS | 1514 | 2.861 | 6.803 | 15.338 | 1.00 | 46.25 |
| ATOM | 391 | CE | LYS | 1514 | 3.268 | 7.796 | 14.261 | 1.00 | 49.76 |
| ATOM | 392 | NZ | LYS | 1514 | 4.304 | 8.771 | 14.705 | 1.00 | 52.14 |
| ATOM | 396 | C | LYS | 1514 | -0.166 | 10.215 | 17.458 | 1.00 | 40.69 |
| ATOM | 397 | O | LYS | 1514 | -1.313 | 9.953 | 17.110 | 1.00 | 41.69 |
| ATOM | 398 | N | MET | 1515 | 0.277 | 11.454 | 17.613 | 1.00 | 43.28 |
| ATOM | 400 | CA | MET | 1515 | -0.569 | 12.610 | 17.379 | 1.00 | 46.21 |
| ATOM | 401 | CB | MET | 1515 | -1.363 | 12.936 | 18.644 | 1.00 | 46.96 |
| ATOM | 402 | CG | MET | 1515 | -0.488 | 13.293 | 19.837 | 1.00 | 47.61 |
| ATOM | 403 | SD | MET | 1515 | -1.413 | 13.464 | 21.358 | 1.00 | 49.77 |
| ATOM | 404 | CE | MET | 1515 | -1.593 | 11.761 | 21.814 | 1.00 | 47.84 |
| ATOM | 405 | C | MET | 1515 | 0.299 | 13.805 | 17.000 | 1.00 | 49.90 |
| ATOM | 406 | O | MET | 1515 | 1.519 | 13.788 | 17.194 | 1.00 | 49.83 |
| ATOM | 407 | N | LEU | 1516 | -0.339 | 14.822 | 16.430 | 1.00 | 54.45 |
| ATOM | 409 | CA | LEU | 1516 | 0.335 | 16.053 | 16.023 | 1.00 | 57.57 |
| ATOM | 410 | CB | LEU | 1516 | -0.483 | 16.762 | 14.944 | 1.00 | 54.10 |
| ATOM | 411 | CG | LEU | 1516 | -0.800 | 16.007 | 13.664 | 1.00 | 50.71 |
| ATOM | 412 | CD1 | LEU | 1516 | -1.830 | 16.800 | 12.901 | 1.00 | 51.20 |
| ATOM | 413 | CD2 | LEU | 1516 | 0.467 | 15.809 | 12.849 | 1.00 | 50.08 |
| ATOM | 414 | C | LEU | 1516 | 0.487 | 17.010 | 17.202 | 1.00 | 61.88 |
| ATOM | 415 | O | LEU | 1516 | -0.170 | 16.852 | 18.235 | 1.00 | 63.30 |
| ATOM | 416 | N | LYS | 1517 | 1.335 | 18.018 | 17.021 | 1.00 | 66.83 |
| ATOM | 418 | CA | LYS | 1517 | 1.568 | 19.036 | 18.037 | 1.00 | 71.46 |
| ATOM | 419 | CB | LYS | 1517 | 2.985 | 19.593 | 17.911 | 1.00 | 76.28 |
| ATOM | 420 | CG | LYS | 1517 | 4.084 | 18.626 | 18.349 | 1.00 | 82.19 |
| ATOM | 421 | CD | LYS | 1517 | 5.450 | 19.085 | 17.846 | 1.00 | 86.93 |
| ATOM | 422 | CE | LYS | 1517 | 6.579 | 18.228 | 18.411 | 1.00 | 90.46 |
| ATOM | 423 | NZ | LYS | 1517 | 7.896 | 18.513 | 17.763 | 1.00 | 92.51 |
| ATOM | 427 | C | LYS | 1517 | 0.549 | 20.156 | 17.837 | 1.00 | 72.44 |
| ATOM | 428 | O | LYS | 1517 | -0.142 | 20.198 | 16.819 | 1.00 | 72.12 |
| ATOM | 429 | N | SER | 1518 | 0.474 | 21.075 | 18.793 | 1.00 | 73.90 |
| ATOM | 431 | CA | SER | 1518 | -0.470 | 22.185 | 18.697 | 1.00 | 74.96 |
| ATOM | 432 | CB | SER | 1518 | -0.498 | 22.980 | 20.002 | 1.00 | 74.72 |
| ATOM | 433 | C | SER | 1518 | -0.133 | 23.100 | 17.525 | 1.00 | 76.16 |
| ATOM | 434 | O | SER | 1518 | -1.029 | 23.667 | 16.897 | 1.00 | 76.56 |
| ATOM | 435 | N | ASP | 1519 | 1.158 | 23.245 | 17.232 | 1.00 | 77.24 |
| ATOM | 437 | CA | ASP | 1519 | 1.601 | 24.094 | 16.125 | 1.00 | 78.51 |
| ATOM | 438 | CB | ASP | 1519 | 2.849 | 24.888 | 16.535 | 1.00 | 79.70 |
| ATOM | 439 | C | ASP | 1519 | 1.887 | 23.264 | 14.865 | 1.00 | 78.29 |
| ATOM | 440 | O | ASP | 1519 | 2.797 | 23.580 | 14.088 | 1.00 | 78.52 |
| ATOM | 441 | N | ALA | 1520 | 1.121 | 22.192 | 14.682 | 1.00 | 76.90 |
| ATOM | 443 | CA | ALA | 1520 | 1.285 | 21.313 | 13.529 | 1.00 | 74.09 |
| ATOM | 444 | CB | ALA | 1520 | 0.737 | 19.930 | 13.840 | 1.00 | 74.20 |
| ATOM | 445 | C | ALA | 1520 | 0.580 | 21.895 | 12.318 | 1.00 | 71.82 |
| ATOM | 446 | O | ALA | 1520 | -0.573 | 22.311 | 12.400 | 1.00 | 71.78 |
| ATOM | 447 | N | THR | 1521 | 1.291 | 21.951 | 11.202 | 1.00 | 69.97 |
| ATOM | 449 | CA | THR | 1521 | 0.734 | 22.480 | 9.970 | 1.00 | 68.86 |
| ATOM | 450 | CB | THR | 1521 | 1.848 | 22.911 | 9.026 | 1.00 | 68.87 |
| ATOM | 451 | OG1 | THR | 1521 | 2.621 | 21.762 | 8.651 | 1.00 | 70.03 |
| ATOM | 453 | CG2 | THR | 1521 | 2.756 | 23.912 | 9.715 | 1.00 | 71.55 |
| ATOM | 454 | C | THR | 1521 | -0.081 | 21.389 | 9.292 | 1.00 | 67.89 |
| ATOM | 455 | O | THR | 1521 | 0.111 | 20.204 | 9.563 | 1.00 | 69.03 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 456 | N | GLU | 1522 | -0.964 | 21.783 | 8.382 | 1.00 | 66.59 |
| ATOM | 458 | CA | GLU | 1522 | -1.785 | 20.821 | 7.657 | 1.00 | 65.71 |
| ATOM | 459 | CB | GLU | 1522 | -2.737 | 21.532 | 6.692 | 1.00 | 65.61 |
| ATOM | 460 | C | GLU | 1522 | -0.886 | 19.823 | 6.909 | 1.00 | 64.32 |
| ATOM | 461 | O | GLU | 1522 | -1.324 | 18.729 | 6.549 | 1.00 | 66.29 |
| ATOM | 462 | N | LYS | 1523 | 0.367 | 20.205 | 6.677 | 1.00 | 59.93 |
| ATOM | 464 | CA | LYS | 1523 | 1.314 | 19.326 | 6.016 | 1.00 | 57.38 |
| ATOM | 465 | CB | LYS | 1523 | 2.629 | 20.064 | 5.747 | 1.00 | 60.47 |
| ATOM | 466 | CG | LYS | 1523 | 3.815 | 19.162 | 5.370 | 1.00 | 62.75 |
| ATOM | 467 | CD | LYS | 1523 | 3.510 | 18.288 | 4.160 | 1.00 | 63.95 |
| ATOM | 468 | CE | LYS | 1523 | 4.759 | 17.596 | 3.652 | 1.00 | 65.88 |
| ATOM | 469 | NZ | LYS | 1523 | 4.429 | 16.721 | 2.494 | 1.00 | 70.37 |
| ATOM | 473 | C | LYS | 1523 | 1.565 | 18.173 | 6.974 | 1.00 | 54.80 |
| ATOM | 474 | O | LYS | 1523 | 1.548 | 17.003 | 6.581 | 1.00 | 54.44 |
| ATOM | 475 | N | ASP | 1524 | 1.786 | 18.523 | 8.239 | 1.00 | 51.67 |
| ATOM | 477 | CA | ASP | 1524 | 2.036 | 17.549 | 9.295 | 1.00 | 49.43 |
| ATOM | 478 | CB | ASP | 1524 | 2.297 | 18.271 | 10.622 | 1.00 | 51.06 |
| ATOM | 479 | CG | ASP | 1524 | 3.598 | 19.080 | 10.613 | 1.00 | 54.03 |
| ATOM | 480 | OD1 | ASP | 1524 | 3.649 | 20.136 | 11.283 | 1.00 | 56.32 |
| ATOM | 481 | OD2 | ASP | 1524 | 4.580 | 18.658 | 9.956 | 1.00 | 56.02 |
| ATOM | 482 | C | ASP | 1524 | 0.847 | 16.596 | 9.413 | 1.00 | 47.73 |
| ATOM | 483 | O | ASP | 1524 | 1.017 | 15.387 | 9.580 | 1.00 | 45.85 |
| ATOM | 484 | N | LEU | 1525 | -0.354 | 17.155 | 9.300 | 1.00 | 47.62 |
| ATOM | 486 | CA | LEU | 1525 | -1.585 | 16.380 | 9.354 | 1.00 | 45.95 |
| ATOM | 487 | CB | LEU | 1525 | -2.801 | 17.307 | 9.271 | 1.00 | 43.61 |
| ATOM | 488 | CG | LEU | 1525 | -4.193 | 16.665 | 9.234 | 1.00 | 44.56 |
| ATOM | 489 | CD1 | LEU | 1525 | -4.364 | 15.543 | 10.268 | 1.00 | 46.02 |
| ATOM | 490 | CD2 | LEU | 1525 | -5.215 | 17.740 | 9.468 | 1.00 | 43.80 |
| ATOM | 491 | C | LEU | 1525 | -1.605 | 15.372 | 8.210 | 1.00 | 45.67 |
| ATOM | 492 | O | LEU | 1525 | -1.921 | 14.204 | 8.416 | 1.00 | 46.78 |
| ATOM | 493 | N | SER | 1526 | -1.245 | 15.822 | 7.014 | 1.00 | 45.44 |
| ATOM | 495 | CA | SER | 1526 | -1.211 | 14.945 | 5.851 | 1.00 | 46.33 |
| ATOM | 496 | CB | SER | 1526 | -0.903 | 15.744 | 4.584 | 1.00 | 48.48 |
| ATOM | 497 | OG | SER | 1526 | -2.012 | 16.546 | 4.218 | 1.00 | 57.28 |
| ATOM | 499 | C | SER | 1526 | -0.192 | 13.821 | 5.995 | 1.00 | 43.84 |
| ATOM | 500 | O | SER | 1526 | -0.480 | 12.669 | 5.674 | 1.00 | 45.24 |
| ATOM | 501 | N | ASP | 1527 | 0.994 | 14.144 | 6.489 | 1.00 | 40.88 |
| ATOM | 503 | CA | ASP | 1527 | 2.024 | 13.128 | 6.646 | 1.00 | 39.70 |
| ATOM | 504 | CB | ASP | 1527 | 3.376 | 13.767 | 6.960 | 1.00 | 37.62 |
| ATOM | 505 | CG | ASP | 1527 | 3.934 | 14.555 | 5.786 | 1.00 | 37.01 |
| ATOM | 506 | OD1 | ASP | 1527 | 3.399 | 14.434 | 4.657 | 1.00 | 35.78 |
| ATOM | 507 | OD2 | ASP | 1527 | 4.916 | 15.295 | 5.992 | 1.00 | 40.23 |
| ATOM | 508 | C | ASP | 1527 | 1.652 | 12.053 | 7.659 | 1.00 | 38.51 |
| ATOM | 509 | O | ASP | 1527 | 1.951 | 10.872 | 7.461 | 1.00 | 37.68 |
| ATOM | 510 | N | LEU | 1528 | 0.973 | 12.460 | 8.725 | 1.00 | 38.16 |
| ATOM | 512 | CA | LEU | 1528 | 0.532 | 11.513 | 9.744 | 1.00 | 38.29 |
| ATOM | 513 | CB | LEU | 1528 | 0.026 | 12.258 | 10.985 | 1.00 | 37.12 |
| ATOM | 514 | CG | LEU | 1528 | -0.505 | 11.412 | 12.153 | 1.00 | 39.03 |
| ATOM | 515 | CD1 | LEU | 1528 | 0.499 | 10.323 | 12.539 | 1.00 | 35.39 |
| ATOM | 516 | CD2 | LEU | 1528 | -0.825 | 12.315 | 13.334 | 1.00 | 35.29 |
| ATOM | 517 | C | LEU | 1528 | -0.568 | 10.611 | 9.155 | 1.00 | 38.10 |
| ATOM | 518 | O | LEU | 1528 | -0.607 | 9.400 | 9.413 | 1.00 | 37.21 |
| ATOM | 519 | N | ILE | 1529 | -1.450 | 11.210 | 8.355 | 1.00 | 36.71 |
| ATOM | 521 | CA | ILE | 1529 | -2.531 | 10.472 | 7.718 | 1.00 | 35.93 |

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ATOM   522   CB    ILE   1529   -3.486   11.419    6.931   1.00   35.67
ATOM   523   CG2   ILE   1529   -4.492   10.619    6.119   1.00   34.04
ATOM   524   CG1   ILE   1529   -4.259   12.295    7.916   1.00   33.81
ATOM   525   CD1   ILE   1529   -5.177   13.288    7.276   1.00   33.58
ATOM   526   C     ILE   1529   -1.912    9.447    6.786   1.00   37.49
ATOM   527   O     ILE   1529   -2.274    8.269    6.829   1.00   37.11
ATOM   528   N     SER   1530   -0.926    9.893    6.003   1.00   38.20
ATOM   530   CA    SER   1530   -0.217    9.036    5.050   1.00   37.49
ATOM   531   CB    SER   1530    0.911    9.822    4.370   1.00   43.32
ATOM   532   OG    SER   1530    0.424   10.970    3.687   1.00   52.31
ATOM   534   C     SER   1530    0.382    7.808    5.719   1.00   34.40
ATOM   535   O     SER   1530    0.234    6.691    5.219   1.00   31.51
ATOM   536   N     GLU   1531    1.048    8.028    6.851   1.00   32.08
ATOM   538   CA    GLU   1531    1.690    6.952    7.594   1.00   30.60
ATOM   539   CB    GLU   1531    2.506    7.515    8.759   1.00   29.70
ATOM   540   CG    GLU   1531    3.094    6.428    9.657   1.00   30.53
ATOM   541   CD    GLU   1531    3.871    6.962   10.839   1.00   33.17
ATOM   542   OE1   GLU   1531    4.473    6.134   11.552   1.00   33.38
ATOM   543   OE2   GLU   1531    3.883    8.193   11.062   1.00   37.52
ATOM   544   C     GLU   1531    0.698    5.911    8.094   1.00   30.17
ATOM   545   O     GLU   1531    0.991    4.714    8.100   1.00   29.76
ATOM   546   N     MET   1532   -0.464    6.379    8.530   1.00   31.34
ATOM   548   CA    MET   1532   -1.521    5.496    9.015   1.00   30.72
ATOM   549   CB    MET   1532   -2.666    6.336    9.591   1.00   29.99
ATOM   550   CG    MET   1532   -3.880    5.523   10.020   1.00   30.10
ATOM   551   SD    MET   1532   -5.173    6.510   10.727   1.00   29.46
ATOM   552   CE    MET   1532   -5.462    7.682    9.455   1.00   23.76
ATOM   553   C     MET   1532   -2.025    4.638    7.843   1.00   30.47
ATOM   554   O     MET   1532   -2.080    3.401    7.925   1.00   27.05
ATOM   555   N     GLU   1533   -2.387    5.319    6.756   1.00   30.56
ATOM   557   CA    GLU   1533   -2.863    4.674    5.542   1.00   30.56
ATOM   558   CB    GLU   1533   -3.090    5.725    4.458   1.00   28.60
ATOM   559   CG    GLU   1533   -4.226    6.677    4.761   1.00   29.08
ATOM   560   CD    GLU   1533   -5.531    5.954    5.014   1.00   31.28
ATOM   561   OE1   GLU   1533   -6.006    5.230    4.117   1.00   33.09
ATOM   562   OE2   GLU   1533   -6.086    6.104    6.121   1.00   34.97
ATOM   563   C     GLU   1533   -1.861    3.638    5.064   1.00   29.86
ATOM   564   O     GLU   1533   -2.232    2.541    4.677   1.00   32.28
ATOM   565   N     MET   1534   -0.590    4.014    5.107   1.00   32.54
ATOM   567   CA    MET   1534    0.515    3.145    4.719   1.00   33.39
ATOM   568   CB    MET   1534    1.826    3.894    4.885   1.00   34.70
ATOM   569   CG    MET   1534    3.038    3.047    4.654   1.00   44.51
ATOM   570   SD    MET   1534    3.479    3.063    2.943   1.00   52.81
ATOM   571   CE    MET   1534    4.349    4.607    2.874   1.00   47.34
ATOM   572   C     MET   1534    0.530    1.896    5.607   1.00   32.98
ATOM   573   O     MET   1534    0.689    0.776    5.115   1.00   34.00
ATOM   574   N     MET   1535    0.364    2.100    6.910   1.00   31.92
ATOM   576   CA    MET   1535    0.336    0.986    7.848   1.00   30.80
ATOM   577   CB    MET   1535    0.252    1.503    9.294   1.00   33.77
ATOM   578   CG    MET   1535    1.509    2.216    9.810   1.00   32.26
ATOM   579   SD    MET   1535    1.520    2.433   11.617   1.00   34.75
ATOM   580   CE    MET   1535    1.183    4.173   11.723   1.00   37.86
ATOM   581   C     MET   1535   -0.837    0.052    7.521   1.00   30.80
ATOM   582   O     MET   1535   -0.704   -1.175    7.589   1.00   32.03
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 583 | N | LYS | 1536 | -1.974 | 0.638 | 7.142 | 1.00 | 31.04 |
| ATOM | 585 | CA | LYS | 1536 | -3.170 | -0.123 | 6.767 | 1.00 | 31.15 |
| ATOM | 586 | CB | LYS | 1536 | -4.334 | 0.808 | 6.415 | 1.00 | 31.21 |
| ATOM | 587 | CG | LYS | 1536 | -4.864 | 1.625 | 7.552 | 1.00 | 27.76 |
| ATOM | 588 | CD | LYS | 1536 | -5.973 | 2.540 | 7.103 | 1.00 | 21.44 |
| ATOM | 589 | CE | LYS | 1536 | -6.434 | 3.401 | 8.248 | 1.00 | 24.69 |
| ATOM | 590 | NZ | LYS | 1536 | -7.578 | 4.241 | 7.868 | 1.00 | 25.84 |
| ATOM | 594 | C | LYS | 1536 | -2.887 | -1.003 | 5.561 | 1.00 | 30.71 |
| ATOM | 595 | O | LYS | 1536 | -3.238 | -2.175 | 5.560 | 1.00 | 34.73 |
| ATOM | 596 | N | MET | 1537 | -2.309 | -0.412 | 4.523 | 1.00 | 31.18 |
| ATOM | 598 | CA | MET | 1537 | -1.967 | -1.148 | 3.307 | 1.00 | 31.53 |
| ATOM | 599 | CB | MET | 1537 | -1.370 | -0.200 | 2.267 | 1.00 | 35.11 |
| ATOM | 600 | CG | MET | 1537 | -2.377 | 0.780 | 1.654 | 1.00 | 42.40 |
| ATOM | 601 | SD | MET | 1537 | -3.657 | -0.051 | 0.685 | 1.00 | 50.10 |
| ATOM | 602 | CE | MET | 1537 | -3.069 | 0.266 | -0.972 | 1.00 | 50.20 |
| ATOM | 603 | C | MET | 1537 | -0.976 | -2.276 | 3.572 | 1.00 | 30.86 |
| ATOM | 604 | O | MET | 1537 | -1.218 | -3.425 | 3.210 | 1.00 | 30.07 |
| ATOM | 605 | N | ILE | 1538 | 0.119 | -1.950 | 4.259 | 1.00 | 30.92 |
| ATOM | 607 | CA | ILE | 1538 | 1.173 | -2.923 | 4.563 | 1.00 | 28.12 |
| ATOM | 608 | CB | ILE | 1538 | 2.359 | -2.254 | 5.313 | 1.00 | 28.71 |
| ATOM | 609 | CG2 | ILE | 1538 | 3.310 | -3.303 | 5.865 | 1.00 | 29.72 |
| ATOM | 610 | CG1 | ILE | 1538 | 3.126 | -1.343 | 4.350 | 1.00 | 30.79 |
| ATOM | 611 | CD1 | ILE | 1538 | 4.375 | -0.745 | 4.945 | 1.00 | 32.46 |
| ATOM | 612 | C | ILE | 1538 | 0.717 | -4.179 | 5.299 | 1.00 | 26.33 |
| ATOM | 613 | O | ILE | 1538 | 1.178 | -5.276 | 4.996 | 1.00 | 24.20 |
| ATOM | 614 | N | GLY | 1539 | -0.188 | -4.027 | 6.258 | 1.00 | 27.41 |
| ATOM | 616 | CA | GLY | 1539 | -0.651 | -5.190 | 6.997 | 1.00 | 27.83 |
| ATOM | 617 | C | GLY | 1539 | 0.240 | -5.533 | 8.179 | 1.00 | 29.10 |
| ATOM | 618 | O | GLY | 1539 | 1.308 | -4.937 | 8.368 | 1.00 | 30.33 |
| ATOM | 619 | N | LYS | 1540 | -0.157 | -6.561 | 8.916 | 1.00 | 29.46 |
| ATOM | 621 | CA | LYS | 1540 | 0.539 | -6.976 | 10.120 | 1.00 | 29.27 |
| ATOM | 622 | CB | LYS | 1540 | -0.470 | -7.520 | 11.139 | 1.00 | 27.01 |
| ATOM | 623 | CG | LYS | 1540 | -1.438 | -6.483 | 11.638 | 1.00 | 29.58 |
| ATOM | 624 | CD | LYS | 1540 | -2.496 | -7.103 | 12.530 | 1.00 | 39.41 |
| ATOM | 625 | CE | LYS | 1540 | -3.548 | -6.069 | 12.952 | 1.00 | 44.14 |
| ATOM | 626 | NZ | LYS | 1540 | -2.994 | -4.996 | 13.828 | 1.00 | 46.92 |
| ATOM | 630 | C | LYS | 1540 | 1.679 | -7.962 | 10.020 | 1.00 | 27.17 |
| ATOM | 631 | O | LYS | 1540 | 1.745 | -8.794 | 9.111 | 1.00 | 26.20 |
| ATOM | 632 | N | HIS | 1541 | 2.565 | -7.856 | 11.006 | 1.00 | 26.96 |
| ATOM | 634 | CA | HIS | 1541 | 3.690 | -8.761 | 11.144 | 1.00 | 27.30 |
| ATOM | 635 | CB | HIS | 1541 | 4.787 | -8.506 | 10.120 | 1.00 | 22.20 |
| ATOM | 636 | CG | HIS | 1541 | 5.849 | -9.555 | 10.125 | 1.00 | 21.32 |
| ATOM | 637 | CD2 | HIS | 1541 | 5.886 | -10.789 | 9.555 | 1.00 | 23.29 |
| ATOM | 638 | ND1 | HIS | 1541 | 7.052 | -9.413 | 10.791 | 1.00 | 19.41 |
| ATOM | 640 | CE1 | HIS | 1541 | 7.775 | -10.509 | 10.633 | 1.00 | 23.61 |
| ATOM | 641 | NE2 | HIS | 1541 | 7.097 | -11.355 | 9.889 | 1.00 | 21.81 |
| ATOM | 643 | C | HIS | 1541 | 4.245 | -8.640 | 12.565 | 1.00 | 28.64 |
| ATOM | 644 | O | HIS | 1541 | 4.290 | -7.549 | 13.132 | 1.00 | 30.64 |
| ATOM | 645 | N | LYS | 1542 | 4.650 | -9.791 | 13.108 | 1.00 | 29.47 |
| ATOM | 647 | CA | LYS | 1542 | 5.200 | -9.893 | 14.457 | 1.00 | 28.78 |
| ATOM | 648 | CB | LYS | 1542 | 5.683 | -11.326 | 14.714 | 1.00 | 30.16 |
| ATOM | 649 | CG | LYS | 1542 | 6.232 | -11.572 | 16.112 | 1.00 | 32.63 |
| ATOM | 650 | CD | LYS | 1542 | 5.277 | -11.046 | 17.155 | 1.00 | 42.90 |
| ATOM | 651 | CE | LYS | 1542 | 5.659 | -11.475 | 18.551 | 1.00 | 48.13 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 652 | NZ | LYS | 1542 | 4.726 | -10.930 | 19.564 | 1.00 | 54.87 |
| ATOM | 656 | C | LYS | 1542 | 6.351 | -8.928 | 14.705 | 1.00 | 26.54 |
| ATOM | 657 | O | LYS | 1542 | 6.440 | -8.321 | 15.773 | 1.00 | 26.19 |
| ATOM | 658 | N | ASN | 1543 | 7.193 | -8.733 | 13.697 | 1.00 | 24.36 |
| ATOM | 660 | CA | ASN | 1543 | 8.357 | -7.874 | 13.852 | 1.00 | 24.08 |
| ATOM | 661 | CB | ASN | 1543 | 9.601 | -8.596 | 13.359 | 1.00 | 22.69 |
| ATOM | 662 | CG | ASN | 1543 | 9.781 | -9.950 | 14.029 | 1.00 | 22.81 |
| ATOM | 663 | OD1 | ASN | 1543 | 9.664 | -10.996 | 13.388 | 1.00 | 23.62 |
| ATOM | 664 | ND2 | ASN | 1543 | 10.028 | -9.938 | 15.324 | 1.00 | 24.94 |
| ATOM | 667 | C | ASN | 1543 | 8.318 | -6.429 | 13.377 | 1.00 | 23.48 |
| ATOM | 668 | O | ASN | 1543 | 9.351 | -5.861 | 13.059 | 1.00 | 22.94 |
| ATOM | 669 | N | ILE | 1544 | 7.130 | -5.821 | 13.380 | 1.00 | 24.15 |
| ATOM | 671 | CA | ILE | 1544 | 6.976 | -4.407 | 13.012 | 1.00 | 24.60 |
| ATOM | 672 | CB | ILE | 1544 | 6.516 | -4.191 | 11.531 | 1.00 | 24.90 |
| ATOM | 673 | CG2 | ILE | 1544 | 7.495 | -4.852 | 10.571 | 1.00 | 21.57 |
| ATOM | 674 | CG1 | ILE | 1544 | 5.081 | -4.688 | 11.316 | 1.00 | 26.66 |
| ATOM | 675 | CD1 | ILE | 1544 | 4.481 | -4.321 | 9.945 | 1.00 | 23.98 |
| ATOM | 676 | C | ILE | 1544 | 5.954 | -3.785 | 13.955 | 1.00 | 24.78 |
| ATOM | 677 | O | ILE | 1544 | 5.160 | -4.503 | 14.558 | 1.00 | 27.87 |
| ATOM | 678 | N | ILE | 1545 | 6.035 | -2.474 | 14.159 | 1.00 | 26.39 |
| ATOM | 680 | CA | ILE | 1545 | 5.089 | -1.779 | 15.025 | 1.00 | 26.79 |
| ATOM | 681 | CB | ILE | 1545 | 5.588 | -0.345 | 15.384 | 1.00 | 28.85 |
| ATOM | 682 | CG2 | ILE | 1545 | 4.512 | 0.449 | 16.103 | 1.00 | 23.60 |
| ATOM | 683 | CG1 | ILE | 1545 | 6.833 | -0.423 | 16.269 | 1.00 | 27.20 |
| ATOM | 684 | CD1 | ILE | 1545 | 6.565 | -0.990 | 17.639 | 1.00 | 27.12 |
| ATOM | 685 | C | ILE | 1545 | 3.792 | -1.708 | 14.224 | 1.00 | 26.99 |
| ATOM | 686 | O | ILE | 1545 | 3.720 | -1.023 | 13.197 | 1.00 | 27.61 |
| ATOM | 687 | N | ASN | 1546 | 2.809 | -2.495 | 14.654 | 1.00 | 26.70 |
| ATOM | 689 | CA | ASN | 1546 | 1.514 | -2.565 | 13.983 | 1.00 | 26.53 |
| ATOM | 690 | CB | ASN | 1546 | 0.871 | -3.953 | 14.169 | 1.00 | 26.23 |
| ATOM | 691 | CG | ASN | 1546 | 1.695 | -5.072 | 13.551 | 1.00 | 24.96 |
| ATOM | 692 | OD1 | ASN | 1546 | 1.773 | -5.206 | 12.330 | 1.00 | 28.08 |
| ATOM | 693 | ND2 | ASN | 1546 | 2.319 | -5.872 | 14.387 | 1.00 | 22.38 |
| ATOM | 696 | C | ASN | 1546 | 0.521 | -1.497 | 14.418 | 1.00 | 26.89 |
| ATOM | 697 | O | ASN | 1546 | 0.610 | -0.952 | 15.523 | 1.00 | 27.40 |
| ATOM | 698 | N | LEU | 1547 | -0.349 | -1.138 | 13.481 | 1.00 | 27.77 |
| ATOM | 700 | CA | LEU | 1547 | -1.416 | -0.175 | 13.701 | 1.00 | 28.28 |
| ATOM | 701 | CB | LEU | 1547 | -1.958 | 0.313 | 12.361 | 1.00 | 27.04 |
| ATOM | 702 | CG | LEU | 1547 | -3.199 | 1.194 | 12.408 | 1.00 | 25.74 |
| ATOM | 703 | CD1 | LEU | 1547 | -2.836 | 2.575 | 12.950 | 1.00 | 27.66 |
| ATOM | 704 | CD2 | LEU | 1547 | -3.799 | 1.289 | 11.014 | 1.00 | 23.38 |
| ATOM | 705 | C | LEU | 1547 | -2.498 | -0.972 | 14.435 | 1.00 | 29.80 |
| ATOM | 706 | O | LEU | 1547 | -2.766 | -2.135 | 14.105 | 1.00 | 28.63 |
| ATOM | 707 | N | LEU | 1548 | -3.088 | -0.351 | 15.448 | 1.00 | 29.91 |
| ATOM | 709 | CA | LEU | 1548 | -4.114 | -0.997 | 16.256 | 1.00 | 28.46 |
| ATOM | 710 | CB | LEU | 1548 | -3.735 | -0.956 | 17.749 | 1.00 | 26.76 |
| ATOM | 711 | CG | LEU | 1548 | -2.460 | -1.701 | 18.162 | 1.00 | 22.44 |
| ATOM | 712 | CD1 | LEU | 1548 | -2.277 | -1.554 | 19.653 | 1.00 | 21.91 |
| ATOM | 713 | CD2 | LEU | 1548 | -2.551 | -3.179 | 17.778 | 1.00 | 20.79 |
| ATOM | 714 | C | LEU | 1548 | -5.480 | -0.365 | 16.058 | 1.00 | 27.31 |
| ATOM | 715 | O | LEU | 1548 | -6.489 | -1.043 | 16.193 | 1.00 | 28.25 |
| ATOM | 716 | N | GLY | 1549 | -5.506 | 0.925 | 15.732 | 1.00 | 24.02 |
| ATOM | 718 | CA | GLY | 1549 | -6.774 | 1.598 | 15.553 | 1.00 | 24.57 |
| ATOM | 719 | C | GLY | 1549 | -6.548 | 3.077 | 15.395 | 1.00 | 25.19 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 720 | O | GLY | 1549 | -5.400 | 3.488 | 15.231 | 1.00 | 28.77 |
| ATOM | 721 | N | ALA | 1550 | -7.617 | 3.875 | 15.427 | 1.00 | 24.66 |
| ATOM | 723 | CA | ALA | 1550 | -7.487 | 5.319 | 15.282 | 1.00 | 24.17 |
| ATOM | 724 | CB | ALA | 1550 | -7.206 | 5.680 | 13.824 | 1.00 | 24.29 |
| ATOM | 725 | C | ALA | 1550 | -8.695 | 6.103 | 15.765 | 1.00 | 23.95 |
| ATOM | 726 | O | ALA | 1550 | -9.810 | 5.590 | 15.780 | 1.00 | 24.95 |
| ATOM | 727 | N | CYS | 1551 | -8.444 | 7.336 | 16.199 | 1.00 | 25.03 |
| ATOM | 729 | CA | CYS | 1551 | -9.482 | 8.270 | 16.639 | 1.00 | 28.21 |
| ATOM | 730 | CB | CYS | 1551 | -9.221 | 8.774 | 18.055 | 1.00 | 26.76 |
| ATOM | 731 | SG | CYS | 1551 | -9.378 | 7.521 | 19.317 | 1.00 | 34.39 |
| ATOM | 732 | C | CYS | 1551 | -9.359 | 9.426 | 15.656 | 1.00 | 29.98 |
| ATOM | 733 | O | CYS | 1551 | -8.482 | 10.281 | 15.800 | 1.00 | 32.14 |
| ATOM | 734 | N | THR | 1552 | -10.198 | 9.412 | 14.625 | 1.00 | 31.09 |
| ATOM | 736 | CA | THR | 1552 | -10.135 | 10.435 | 13.595 | 1.00 | 32.91 |
| ATOM | 737 | CB | THR | 1552 | -10.052 | 9.781 | 12.189 | 1.00 | 32.60 |
| ATOM | 738 | OG1 | THR | 1552 | -11.276 | 9.097 | 11.890 | 1.00 | 32.12 |
| ATOM | 740 | CG2 | THR | 1552 | -8.928 | 8.768 | 12.144 | 1.00 | 32.74 |
| ATOM | 741 | C | THR | 1552 | -11.282 | 11.419 | 13.591 | 1.00 | 35.26 |
| ATOM | 742 | O | THR | 1552 | -11.171 | 12.525 | 13.057 | 1.00 | 35.10 |
| ATOM | 743 | N | GLN | 1553 | -12.397 | 11.014 | 14.179 | 1.00 | 39.01 |
| ATOM | 745 | CA | GLN | 1553 | -13.585 | 11.846 | 14.180 | 1.00 | 41.97 |
| ATOM | 746 | CB | GLN | 1553 | -14.832 | 10.968 | 14.020 | 1.00 | 41.17 |
| ATOM | 747 | CG | GLN | 1553 | -14.915 | 10.238 | 12.672 | 1.00 | 39.06 |
| ATOM | 748 | CD | GLN | 1553 | -14.900 | 11.200 | 11.496 | 1.00 | 41.84 |
| ATOM | 749 | OE1 | GLN | 1553 | -15.785 | 12.045 | 11.359 | 1.00 | 41.92 |
| ATOM | 750 | NE2 | GLN | 1553 | -13.876 | 11.090 | 10.652 | 1.00 | 42.33 |
| ATOM | 753 | C | GLN | 1553 | -13.727 | 12.777 | 15.372 | 1.00 | 45.35 |
| ATOM | 754 | O | GLN | 1553 | -13.358 | 12.423 | 16.489 | 1.00 | 47.02 |
| ATOM | 755 | N | ASP | 1554 | -14.225 | 13.981 | 15.090 | 1.00 | 48.60 |
| ATOM | 757 | CA | ASP | 1554 | -14.479 | 15.016 | 16.084 | 1.00 | 50.64 |
| ATOM | 758 | CB | ASP | 1554 | -15.832 | 14.766 | 16.758 | 1.00 | 54.52 |
| ATOM | 759 | CG | ASP | 1554 | -17.003 | 14.955 | 15.809 | 1.00 | 60.54 |
| ATOM | 760 | OD1 | ASP | 1554 | -18.072 | 15.409 | 16.274 | 1.00 | 66.04 |
| ATOM | 761 | OD2 | ASP | 1554 | -16.860 | 14.661 | 14.601 | 1.00 | 65.09 |
| ATOM | 762 | C | ASP | 1554 | -13.395 | 15.173 | 17.133 | 1.00 | 49.89 |
| ATOM | 763 | O | ASP | 1554 | -13.611 | 14.879 | 18.310 | 1.00 | 51.48 |
| ATOM | 764 | N | GLY | 1555 | -12.232 | 15.643 | 16.699 | 1.00 | 48.40 |
| ATOM | 766 | CA | GLY | 1555 | -11.131 | 15.834 | 17.617 | 1.00 | 46.16 |
| ATOM | 767 | C | GLY | 1555 | -9.798 | 15.626 | 16.935 | 1.00 | 44.64 |
| ATOM | 768 | O | GLY | 1555 | -9.737 | 15.581 | 15.716 | 1.00 | 45.22 |
| ATOM | 769 | N | PRO | 1556 | -8.708 | 15.525 | 17.702 | 1.00 | 44.68 |
| ATOM | 770 | CD | PRO | 1556 | -8.672 | 15.683 | 19.164 | 1.00 | 45.39 |
| ATOM | 771 | CA | PRO | 1556 | -7.359 | 15.326 | 17.177 | 1.00 | 42.95 |
| ATOM | 772 | CB | PRO | 1556 | -6.484 | 15.549 | 18.411 | 1.00 | 43.74 |
| ATOM | 773 | CG | PRO | 1556 | -7.354 | 16.347 | 19.345 | 1.00 | 47.32 |
| ATOM | 774 | C | PRO | 1556 | -7.164 | 13.912 | 16.665 | 1.00 | 42.34 |
| ATOM | 775 | O | PRO | 1556 | -7.636 | 12.953 | 17.287 | 1.00 | 42.75 |
| ATOM | 776 | N | LEU | 1557 | -6.451 | 13.788 | 15.547 | 1.00 | 39.83 |
| ATOM | 778 | CA | LEU | 1557 | -6.169 | 12.490 | 14.954 | 1.00 | 36.64 |
| ATOM | 779 | CB | LEU | 1557 | -5.496 | 12.669 | 13.587 | 1.00 | 34.49 |
| ATOM | 780 | CG | LEU | 1557 | -5.009 | 11.404 | 12.870 | 1.00 | 31.29 |
| ATOM | 781 | CD1 | LEU | 1557 | -6.169 | 10.436 | 12.628 | 1.00 | 27.86 |
| ATOM | 782 | CD2 | LEU | 1557 | -4.314 | 11.775 | 11.570 | 1.00 | 25.40 |
| ATOM | 783 | C | LEU | 1557 | -5.244 | 11.732 | 15.894 | 1.00 | 35.44 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 784 | O | LEU | 1557 | -4.210 | 12.264 | 16.316 | 1.00 | 36.12 |
| ATOM | 785 | N | TYR | 1558 | -5.664 | 10.539 | 16.292 | 1.00 | 32.49 |
| ATOM | 787 | CA | TYR | 1558 | -4.861 | 9.697 | 17.157 | 1.00 | 31.87 |
| ATOM | 788 | CB | TYR | 1558 | -5.590 | 9.348 | 18.470 | 1.00 | 33.93 |
| ATOM | 789 | CG | TYR | 1558 | -5.695 | 10.476 | 19.471 | 1.00 | 35.34 |
| ATOM | 790 | CD1 | TYR | 1558 | -6.566 | 10.394 | 20.565 | 1.00 | 37.12 |
| ATOM | 791 | CE1 | TYR | 1558 | -6.683 | 11.456 | 21.479 | 1.00 | 36.44 |
| ATOM | 792 | CD2 | TYR | 1558 | -4.945 | 11.636 | 19.317 | 1.00 | 37.27 |
| ATOM | 793 | CE2 | TYR | 1558 | -5.054 | 12.690 | 20.213 | 1.00 | 39.62 |
| ATOM | 794 | CZ | TYR | 1558 | -5.921 | 12.598 | 21.289 | 1.00 | 40.05 |
| ATOM | 795 | OH | TYR | 1558 | -6.008 | 13.668 | 22.155 | 1.00 | 44.98 |
| ATOM | 797 | C | TYR | 1558 | -4.600 | 8.419 | 16.387 | 1.00 | 31.58 |
| ATOM | 798 | O | TYR | 1558 | -5.532 | 7.750 | 15.936 | 1.00 | 30.22 |
| ATOM | 799 | N | VAL | 1559 | -3.331 | 8.129 | 16.153 | 1.00 | 33.43 |
| ATOM | 801 | CA | VAL | 1559 | -2.947 | 6.907 | 15.463 | 1.00 | 31.42 |
| ATOM | 802 | CB | VAL | 1559 | -1.849 | 7.160 | 14.419 | 1.00 | 32.31 |
| ATOM | 803 | CG1 | VAL | 1559 | -1.516 | 5.851 | 13.675 | 1.00 | 26.79 |
| ATOM | 804 | CG2 | VAL | 1559 | -2.308 | 8.265 | 13.453 | 1.00 | 30.63 |
| ATOM | 805 | C | VAL | 1559 | -2.438 | 5.979 | 16.556 | 1.00 | 28.67 |
| ATOM | 806 | O | VAL | 1559 | -1.393 | 6.223 | 17.155 | 1.00 | 30.08 |
| ATOM | 807 | N | ILE | 1560 | -3.230 | 4.960 | 16.852 | 1.00 | 25.80 |
| ATOM | 809 | CA | ILE | 1560 | -2.915 | 3.998 | 17.894 | 1.00 | 25.33 |
| ATOM | 810 | CB | ILE | 1560 | -4.219 | 3.443 | 18.506 | 1.00 | 22.34 |
| ATOM | 811 | CG2 | ILE | 1560 | -3.931 | 2.695 | 19.784 | 1.00 | 20.36 |
| ATOM | 812 | CG1 | ILE | 1560 | -5.172 | 4.603 | 18.809 | 1.00 | 21.34 |
| ATOM | 813 | CD1 | ILE | 1560 | -6.583 | 4.190 | 19.093 | 1.00 | 20.68 |
| ATOM | 814 | C | ILE | 1560 | -2.073 | 2.857 | 17.341 | 1.00 | 27.16 |
| ATOM | 815 | O | ILE | 1560 | -2.520 | 2.116 | 16.455 | 1.00 | 29.67 |
| ATOM | 816 | N | VAL | 1561 | -0.858 | 2.714 | 17.860 | 1.00 | 27.69 |
| ATOM | 818 | CA | VAL | 1561 | 0.060 | 1.667 | 17.411 | 1.00 | 28.27 |
| ATOM | 819 | CB | VAL | 1561 | 1.311 | 2.269 | 16.696 | 1.00 | 27.34 |
| ATOM | 820 | CG1 | VAL | 1561 | 0.892 | 3.019 | 15.445 | 1.00 | 21.76 |
| ATOM | 821 | CG2 | VAL | 1561 | 2.074 | 3.201 | 17.639 | 1.00 | 26.00 |
| ATOM | 822 | C | VAL | 1561 | 0.509 | 0.809 | 18.588 | 1.00 | 28.70 |
| ATOM | 823 | O | VAL | 1561 | 0.221 | 1.139 | 19.746 | 1.00 | 30.52 |
| ATOM | 824 | N | GLU | 1562 | 1.166 | -0.311 | 18.286 | 1.00 | 28.64 |
| ATOM | 826 | CA | GLU | 1562 | 1.658 | -1.220 | 19.318 | 1.00 | 27.77 |
| ATOM | 827 | CB | GLU | 1562 | 2.278 | -2.465 | 18.693 | 1.00 | 24.57 |
| ATOM | 828 | CG | GLU | 1562 | 1.251 | -3.452 | 18.208 | 1.00 | 24.76 |
| ATOM | 829 | CD | GLU | 1562 | 1.864 | -4.641 | 17.501 | 1.00 | 27.27 |
| ATOM | 830 | OE1 | GLU | 1562 | 1.272 | -5.739 | 17.580 | 1.00 | 28.27 |
| ATOM | 831 | OE2 | GLU | 1562 | 2.920 | -4.487 | 16.849 | 1.00 | 29.25 |
| ATOM | 832 | C | GLU | 1562 | 2.674 | -0.538 | 20.217 | 1.00 | 28.79 |
| ATOM | 833 | O | GLU | 1562 | 3.453 | 0.292 | 19.760 | 1.00 | 29.38 |
| ATOM | 834 | N | TYR | 1563 | 2.627 | -0.871 | 21.503 | 1.00 | 30.84 |
| ATOM | 836 | CA | TYR | 1563 | 3.534 | -0.304 | 22.493 | 1.00 | 31.43 |
| ATOM | 837 | CB | TYR | 1563 | 2.782 | -0.088 | 23.799 | 1.00 | 32.10 |
| ATOM | 838 | CG | TYR | 1563 | 3.632 | 0.376 | 24.952 | 1.00 | 33.93 |
| ATOM | 839 | CD1 | TYR | 1563 | 4.366 | 1.552 | 24.873 | 1.00 | 34.85 |
| ATOM | 840 | CE1 | TYR | 1563 | 5.140 | 1.992 | 25.947 | 1.00 | 37.53 |
| ATOM | 841 | CD2 | TYR | 1563 | 3.683 | -0.356 | 26.136 | 1.00 | 34.81 |
| ATOM | 842 | CE2 | TYR | 1563 | 4.452 | 0.072 | 27.211 | 1.00 | 34.01 |
| ATOM | 843 | CZ | TYR | 1563 | 5.173 | 1.245 | 27.113 | 1.00 | 35.79 |
| ATOM | 844 | OH | TYR | 1563 | 5.920 | 1.677 | 28.184 | 1.00 | 39.10 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 846 | C | TYR | 1563 | 4.767 | -1.166 | 22.731 | 1.00 | 31.38 |
| ATOM | 847 | O | TYR | 1563 | 4.672 | -2.385 | 22.905 | 1.00 | 30.73 |
| ATOM | 848 | N | ALA | 1564 | 5.930 | -0.525 | 22.725 | 1.00 | 32.23 |
| ATOM | 850 | CA | ALA | 1564 | 7.198 | -1.212 | 22.953 | 1.00 | 35.90 |
| ATOM | 851 | CB | ALA | 1564 | 8.178 | -0.866 | 21.833 | 1.00 | 36.44 |
| ATOM | 852 | C | ALA | 1564 | 7.711 | -0.719 | 24.307 | 1.00 | 36.52 |
| ATOM | 853 | O | ALA | 1564 | 8.332 | 0.349 | 24.403 | 1.00 | 39.16 |
| ATOM | 854 | N | SER | 1565 | 7.424 | -1.482 | 25.359 | 1.00 | 34.62 |
| ATOM | 856 | CA | SER | 1565 | 7.801 | -1.071 | 26.700 | 1.00 | 34.91 |
| ATOM | 857 | CB | SER | 1565 | 7.124 | -1.945 | 27.750 | 1.00 | 32.11 |
| ATOM | 858 | OG | SER | 1565 | 7.606 | -3.271 | 27.696 | 1.00 | 32.92 |
| ATOM | 860 | C | SER | 1565 | 9.288 | -0.968 | 26.996 | 1.00 | 35.56 |
| ATOM | 861 | O | SER | 1565 | 9.674 | -0.219 | 27.886 | 1.00 | 38.69 |
| ATOM | 862 | N | LYS | 1566 | 10.127 | -1.673 | 26.243 | 1.00 | 33.70 |
| ATOM | 864 | CA | LYS | 1566 | 11.557 | -1.625 | 26.526 | 1.00 | 31.40 |
| ATOM | 865 | CB | LYS | 1566 | 12.137 | -3.033 | 26.530 | 1.00 | 30.56 |
| ATOM | 866 | CG | LYS | 1566 | 11.555 | -3.869 | 27.664 | 1.00 | 32.32 |
| ATOM | 867 | CD | LYS | 1566 | 11.997 | -5.308 | 27.599 | 1.00 | 36.47 |
| ATOM | 868 | CE | LYS | 1566 | 11.632 | -6.031 | 28.872 | 1.00 | 36.97 |
| ATOM | 869 | NZ | LYS | 1566 | 12.104 | -7.436 | 28.804 | 1.00 | 41.62 |
| ATOM | 873 | C | LYS | 1566 | 12.380 | -0.664 | 25.683 | 1.00 | 32.18 |
| ATOM | 874 | O | LYS | 1566 | 13.616 | -0.691 | 25.715 | 1.00 | 32.57 |
| ATOM | 875 | N | GLY | 1567 | 11.686 | 0.223 | 24.973 | 1.00 | 33.39 |
| ATOM | 877 | CA | GLY | 1567 | 12.345 | 1.224 | 24.156 | 1.00 | 32.13 |
| ATOM | 878 | C | GLY | 1567 | 13.074 | 0.719 | 22.928 | 1.00 | 31.70 |
| ATOM | 879 | O | GLY | 1567 | 12.912 | -0.430 | 22.530 | 1.00 | 33.30 |
| ATOM | 880 | N | ASN | 1568 | 13.883 | 1.589 | 22.331 | 1.00 | 31.08 |
| ATOM | 882 | CA | ASN | 1568 | 14.632 | 1.230 | 21.139 | 1.00 | 31.00 |
| ATOM | 883 | CB | ASN | 1568 | 15.066 | 2.478 | 20.365 | 1.00 | 31.30 |
| ATOM | 884 | CG | ASN | 1568 | 16.127 | 3.271 | 21.074 | 1.00 | 30.47 |
| ATOM | 885 | OD1 | ASN | 1568 | 17.130 | 2.733 | 21.508 | 1.00 | 32.19 |
| ATOM | 886 | ND2 | ASN | 1568 | 15.934 | 4.580 | 21.144 | 1.00 | 32.13 |
| ATOM | 889 | C | ASN | 1568 | 15.802 | 0.295 | 21.393 | 1.00 | 30.62 |
| ATOM | 890 | O | ASN | 1568 | 16.357 | 0.256 | 22.483 | 1.00 | 32.91 |
| ATOM | 891 | N | LEU | 1569 | 16.193 | -0.428 | 20.354 | 1.00 | 30.92 |
| ATOM | 893 | CA | LEU | 1569 | 17.269 | -1.403 | 20.417 | 1.00 | 31.22 |
| ATOM | 894 | CB | LEU | 1569 | 17.418 | -2.083 | 19.054 | 1.00 | 29.57 |
| ATOM | 895 | CG | LEU | 1569 | 18.415 | -3.231 | 18.893 | 1.00 | 29.22 |
| ATOM | 896 | CD1 | LEU | 1569 | 18.284 | -4.261 | 20.024 | 1.00 | 21.30 |
| ATOM | 897 | CD2 | LEU | 1569 | 18.184 | -3.863 | 17.523 | 1.00 | 24.99 |
| ATOM | 898 | C | LEU | 1569 | 18.609 | -0.838 | 20.878 | 1.00 | 32.44 |
| ATOM | 899 | O | LEU | 1569 | 19.328 | -1.499 | 21.618 | 1.00 | 33.12 |
| ATOM | 900 | N | ARG | 1570 | 18.954 | 0.370 | 20.432 | 1.00 | 33.24 |
| ATOM | 902 | CA | ARG | 1570 | 20.218 | 0.983 | 20.834 | 1.00 | 33.01 |
| ATOM | 903 | CB | ARG | 1570 | 20.348 | 2.394 | 20.256 | 1.00 | 32.36 |
| ATOM | 904 | CG | ARG | 1570 | 21.586 | 3.129 | 20.758 | 1.00 | 38.28 |
| ATOM | 905 | CD | ARG | 1570 | 21.672 | 4.538 | 20.221 | 1.00 | 41.93 |
| ATOM | 906 | NE | ARG | 1570 | 20.428 | 5.278 | 20.412 | 1.00 | 49.82 |
| ATOM | 908 | CZ | ARG | 1570 | 19.975 | 5.721 | 21.584 | 1.00 | 52.37 |
| ATOM | 909 | NH1 | ARG | 1570 | 20.659 | 5.510 | 22.712 | 1.00 | 51.61 |
| ATOM | 912 | NH2 | ARG | 1570 | 18.824 | 6.377 | 21.622 | 1.00 | 53.28 |
| ATOM | 915 | C | ARG | 1570 | 20.308 | 1.023 | 22.371 | 1.00 | 33.90 |
| ATOM | 916 | O | ARG | 1570 | 21.184 | 0.391 | 22.970 | 1.00 | 33.17 |
| ATOM | 917 | N | GLU | 1571 | 19.359 | 1.730 | 22.981 | 1.00 | 33.45 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 919 | CA | GLU | 1571 | 19.284 | 1.861 | 24.432 | 1.00 | 34.87 |
| ATOM | 920 | CB | GLU | 1571 | 18.052 | 2.688 | 24.794 | 1.00 | 35.83 |
| ATOM | 921 | CG | GLU | 1571 | 18.158 | 4.145 | 24.354 | 1.00 | 41.61 |
| ATOM | 922 | CD | GLU | 1571 | 16.814 | 4.870 | 24.318 | 1.00 | 47.33 |
| ATOM | 923 | OE1 | GLU | 1571 | 15.759 | 4.199 | 24.362 | 1.00 | 50.68 |
| ATOM | 924 | OE2 | GLU | 1571 | 16.812 | 6.120 | 24.218 | 1.00 | 48.07 |
| ATOM | 925 | C | GLU | 1571 | 19.223 | 0.487 | 25.098 | 1.00 | 34.39 |
| ATOM | 926 | O | GLU | 1571 | 19.968 | 0.202 | 26.041 | 1.00 | 34.04 |
| ATOM | 927 | N | TYR | 1572 | 18.363 | -0.376 | 24.572 | 1.00 | 33.49 |
| ATOM | 929 | CA | TYR | 1572 | 18.204 | -1.728 | 25.083 | 1.00 | 30.45 |
| ATOM | 930 | CB | TYR | 1572 | 17.210 | -2.495 | 24.202 | 1.00 | 28.13 |
| ATOM | 931 | CG | TYR | 1572 | 17.074 | -3.971 | 24.487 | 1.00 | 25.80 |
| ATOM | 932 | CD1 | TYR | 1572 | 16.105 | -4.443 | 25.371 | 1.00 | 28.92 |
| ATOM | 933 | CE1 | TYR | 1572 | 15.954 | -5.804 | 25.618 | 1.00 | 30.03 |
| ATOM | 934 | CD2 | TYR | 1572 | 17.899 | -4.899 | 23.863 | 1.00 | 24.61 |
| ATOM | 935 | CE2 | TYR | 1572 | 17.760 | -6.260 | 24.102 | 1.00 | 26.05 |
| ATOM | 936 | CZ | TYR | 1572 | 16.790 | -6.705 | 24.982 | 1.00 | 29.23 |
| ATOM | 937 | OH | TYR | 1572 | 16.651 | -8.052 | 25.227 | 1.00 | 33.74 |
| ATOM | 939 | C | TYR | 1572 | 19.549 | -2.447 | 25.113 | 1.00 | 31.30 |
| ATOM | 940 | O | TYR | 1572 | 19.880 | -3.126 | 26.090 | 1.00 | 32.43 |
| ATOM | 941 | N | LEU | 1573 | 20.334 | -2.266 | 24.058 | 1.00 | 29.68 |
| ATOM | 943 | CA | LEU | 1573 | 21.625 | -2.923 | 23.972 | 1.00 | 30.04 |
| ATOM | 944 | CB | LEU | 1573 | 22.145 | -2.909 | 22.529 | 1.00 | 26.13 |
| ATOM | 945 | CG | LEU | 1573 | 21.532 | -3.870 | 21.490 | 1.00 | 25.24 |
| ATOM | 946 | CD1 | LEU | 1573 | 22.097 | -3.563 | 20.113 | 1.00 | 19.70 |
| ATOM | 947 | CD2 | LEU | 1573 | 21.807 | -5.317 | 21.839 | 1.00 | 22.05 |
| ATOM | 948 | C | LEU | 1573 | 22.645 | -2.308 | 24.927 | 1.00 | 34.47 |
| ATOM | 949 | O | LEU | 1573 | 23.354 | -3.031 | 25.644 | 1.00 | 34.95 |
| ATOM | 950 | N | GLN | 1574 | 22.691 | -0.980 | 24.978 | 1.00 | 35.47 |
| ATOM | 952 | CA | GLN | 1574 | 23.639 | -0.293 | 25.850 | 1.00 | 37.09 |
| ATOM | 953 | CB | GLN | 1574 | 23.601 | 1.206 | 25.579 | 1.00 | 36.70 |
| ATOM | 954 | CG | GLN | 1574 | 24.033 | 1.559 | 24.171 | 1.00 | 39.77 |
| ATOM | 955 | CD | GLN | 1574 | 23.960 | 3.045 | 23.884 | 1.00 | 41.51 |
| ATOM | 956 | OE1 | GLN | 1574 | 23.592 | 3.837 | 24.751 | 1.00 | 42.57 |
| ATOM | 957 | NE2 | GLN | 1574 | 24.288 | 3.431 | 22.652 | 1.00 | 41.34 |
| ATOM | 960 | C | GLN | 1574 | 23.400 | -0.588 | 27.332 | 1.00 | 37.85 |
| ATOM | 961 | O | GLN | 1574 | 24.343 | -0.801 | 28.090 | 1.00 | 38.87 |
| ATOM | 962 | N | ALA | 1575 | 22.131 | -0.667 | 27.720 | 1.00 | 39.01 |
| ATOM | 964 | CA | ALA | 1575 | 21.740 | -0.944 | 29.098 | 1.00 | 37.00 |
| ATOM | 965 | CB | ALA | 1575 | 20.261 | -0.678 | 29.273 | 1.00 | 35.71 |
| ATOM | 966 | C | ALA | 1575 | 22.061 | -2.359 | 29.559 | 1.00 | 39.14 |
| ATOM | 967 | O | ALA | 1575 | 21.839 | -2.692 | 30.719 | 1.00 | 43.81 |
| ATOM | 968 | N | ARG | 1576 | 22.563 | -3.201 | 28.665 | 1.00 | 38.39 |
| ATOM | 970 | CA | ARG | 1576 | 22.897 | -4.568 | 29.032 | 1.00 | 37.71 |
| ATOM | 971 | CB | ARG | 1576 | 21.994 | -5.544 | 28.290 | 1.00 | 38.26 |
| ATOM | 972 | CG | ARG | 1576 | 20.555 | -5.383 | 28.700 | 1.00 | 38.00 |
| ATOM | 973 | CD | ARG | 1576 | 19.653 | -6.282 | 27.920 | 1.00 | 34.74 |
| ATOM | 974 | NE | ARG | 1576 | 18.279 | -6.190 | 28.388 | 1.00 | 32.88 |
| ATOM | 976 | CZ | ARG | 1576 | 17.572 | -5.066 | 28.442 | 1.00 | 34.02 |
| ATOM | 977 | NH1 | ARG | 1576 | 18.114 | -3.913 | 28.068 | 1.00 | 35.57 |
| ATOM | 980 | NH2 | ARG | 1576 | 16.298 | -5.102 | 28.800 | 1.00 | 36.71 |
| ATOM | 983 | C | ARG | 1576 | 24.365 | -4.927 | 28.828 | 1.00 | 39.59 |
| ATOM | 984 | O | ARG | 1576 | 24.735 | -6.113 | 28.788 | 1.00 | 39.83 |
| ATOM | 985 | N | ARG | 1577 | 25.200 | -3.900 | 28.687 | 1.00 | 38.82 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 987 | CA | ARG | 1577 | 26.631 | -4.101 | 28.520 | 1.00 | 39.07 |
| ATOM | 988 | CB | ARG | 1577 | 27.310 | -2.797 | 28.090 | 1.00 | 34.91 |
| ATOM | 989 | CG | ARG | 1577 | 27.033 | -2.323 | 26.681 | 1.00 | 33.87 |
| ATOM | 990 | CD | ARG | 1577 | 27.730 | -0.981 | 26.428 | 1.00 | 33.06 |
| ATOM | 991 | NE | ARG | 1577 | 27.722 | -0.612 | 25.015 | 1.00 | 38.87 |
| ATOM | 993 | CZ | ARG | 1577 | 28.174 | 0.538 | 24.517 | 1.00 | 39.76 |
| ATOM | 994 | NH1 | ARG | 1577 | 28.683 | 1.470 | 25.305 | 1.00 | 40.68 |
| ATOM | 997 | NH2 | ARG | 1577 | 28.122 | 0.758 | 23.213 | 1.00 | 43.26 |
| ATOM | 1000 | C | ARG | 1577 | 27.181 | -4.501 | 29.885 | 1.00 | 41.58 |
| ATOM | 1001 | O | ARG | 1577 | 26.586 | -4.181 | 30.917 | 1.00 | 42.48 |
| ATOM | 1002 | N | PRO | 1578 | 28.294 | -5.249 | 29.919 | 1.00 | 43.07 |
| ATOM | 1003 | CD | PRO | 1578 | 29.110 | -5.812 | 28.823 | 1.00 | 43.36 |
| ATOM | 1004 | CA | PRO | 1578 | 28.839 | -5.626 | 31.223 | 1.00 | 42.69 |
| ATOM | 1005 | CB | PRO | 1578 | 29.966 | -6.595 | 30.857 | 1.00 | 42.22 |
| ATOM | 1006 | CG | PRO | 1578 | 30.412 | -6.103 | 29.516 | 1.00 | 43.64 |
| ATOM | 1007 | C | PRO | 1578 | 29.366 | -4.350 | 31.882 | 1.00 | 43.37 |
| ATOM | 1008 | O | PRO | 1578 | 29.530 | -3.319 | 31.215 | 1.00 | 42.50 |
| ATOM | 1009 | N | PRO | 1579 | 29.596 | -4.380 | 33.198 | 1.00 | 45.24 |
| ATOM | 1010 | CD | PRO | 1579 | 29.279 | -5.435 | 34.174 | 1.00 | 44.69 |
| ATOM | 1011 | CA | PRO | 1579 | 30.099 | -3.187 | 33.882 | 1.00 | 46.27 |
| ATOM | 1012 | CB | PRO | 1579 | 29.979 | -3.567 | 35.353 | 1.00 | 45.78 |
| ATOM | 1013 | CG | PRO | 1579 | 28.894 | -4.615 | 35.361 | 1.00 | 46.15 |
| ATOM | 1014 | C | PRO | 1579 | 31.548 | -2.869 | 33.500 | 1.00 | 48.38 |
| ATOM | 1015 | O | PRO | 1579 | 32.410 | -3.753 | 33.478 | 1.00 | 50.64 |
| ATOM | 1016 | N | GLU | 1592 | 19.022 | -5.398 | 32.495 | 1.00 | 65.98 |
| ATOM | 1018 | CA | GLU | 1592 | 20.442 | -5.048 | 32.492 | 1.00 | 64.80 |
| ATOM | 1019 | CB | GLU | 1592 | 20.796 | -4.241 | 33.740 | 1.00 | 67.30 |
| ATOM | 1020 | C | GLU | 1592 | 21.351 | -6.275 | 32.371 | 1.00 | 63.80 |
| ATOM | 1021 | O | GLU | 1592 | 22.545 | -6.149 | 32.089 | 1.00 | 65.21 |
| ATOM | 1022 | N | GLU | 1593 | 20.789 | -7.458 | 32.607 | 1.00 | 61.44 |
| ATOM | 1024 | CA | GLU | 1593 | 21.560 | -8.691 | 32.495 | 1.00 | 60.82 |
| ATOM | 1025 | CB | GLU | 1593 | 20.681 | -9.899 | 32.807 | 1.00 | 61.47 |
| ATOM | 1026 | C | GLU | 1593 | 22.144 | -8.803 | 31.089 | 1.00 | 59.12 |
| ATOM | 1027 | O | GLU | 1593 | 21.468 | -8.525 | 30.097 | 1.00 | 59.49 |
| ATOM | 1028 | N | GLN | 1594 | 23.408 | -9.201 | 31.017 | 1.00 | 57.33 |
| ATOM | 1030 | CA | GLN | 1594 | 24.103 | -9.334 | 29.744 | 1.00 | 55.30 |
| ATOM | 1031 | CB | GLN | 1594 | 25.523 | -9.880 | 29.957 | 1.00 | 54.87 |
| ATOM | 1032 | CG | GLN | 1594 | 26.438 | -8.959 | 30.757 | 1.00 | 53.34 |
| ATOM | 1033 | CD | GLN | 1594 | 27.704 | -9.660 | 31.248 | 1.00 | 55.27 |
| ATOM | 1034 | OE1 | GLN | 1594 | 28.256 | -10.536 | 30.572 | 1.00 | 56.47 |
| ATOM | 1035 | NE2 | GLN | 1594 | 28.166 | -9.275 | 32.434 | 1.00 | 51.46 |
| ATOM | 1038 | C | GLN | 1594 | 23.336 | -10.229 | 28.781 | 1.00 | 52.29 |
| ATOM | 1039 | O | GLN | 1594 | 22.648 | -11.166 | 29.190 | 1.00 | 52.56 |
| ATOM | 1040 | N | LEU | 1595 | 23.447 | -9.913 | 27.499 | 1.00 | 49.40 |
| ATOM | 1042 | CA | LEU | 1595 | 22.783 | -10.676 | 26.455 | 1.00 | 46.00 |
| ATOM | 1043 | CB | LEU | 1595 | 22.452 | -9.760 | 25.274 | 1.00 | 42.94 |
| ATOM | 1044 | CG | LEU | 1595 | 21.390 | -8.711 | 25.626 | 1.00 | 43.90 |
| ATOM | 1045 | CD1 | LEU | 1595 | 21.495 | -7.484 | 24.743 | 1.00 | 39.46 |
| ATOM | 1046 | CD2 | LEU | 1595 | 20.005 | -9.347 | 25.569 | 1.00 | 41.86 |
| ATOM | 1047 | C | LEU | 1595 | 23.741 | -11.762 | 26.029 | 1.00 | 43.96 |
| ATOM | 1048 | O | LEU | 1595 | 24.950 | -11.550 | 26.043 | 1.00 | 44.24 |
| ATOM | 1049 | N | SER | 1596 | 23.217 | -12.941 | 25.714 | 1.00 | 43.29 |
| ATOM | 1051 | CA | SER | 1596 | 24.076 | -14.027 | 25.275 | 1.00 | 42.40 |
| ATOM | 1052 | CB | SER | 1596 | 23.388 | -15.374 | 25.484 | 1.00 | 41.83 |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1053 | OG | SER | 1596 | 22.218 | -15.483 | 24.697 | 1.00 | 44.25 | |
| ATOM | 1055 | C | SER | 1596 | 24.392 | -13.817 | 23.800 | 1.00 | 42.64 | |
| ATOM | 1056 | O | SER | 1596 | 23.857 | -12.900 | 23.171 | 1.00 | 43.14 | |
| ATOM | 1057 | N | SER | 1597 | 25.277 | -14.645 | 23.255 | 1.00 | 42.59 | |
| ATOM | 1059 | CA | SER | 1597 | 25.629 | -14.553 | 21.850 | 1.00 | 42.91 | |
| ATOM | 1060 | CB | SER | 1597 | 26.739 | -15.547 | 21.516 | 1.00 | 45.26 | |
| ATOM | 1061 | OG | SER | 1597 | 27.812 | -15.436 | 22.431 | 1.00 | 56.41 | |
| ATOM | 1063 | C | SER | 1597 | 24.380 | -14.909 | 21.048 | 1.00 | 42.35 | |
| ATOM | 1064 | O | SER | 1597 | 24.113 | -14.322 | 20.003 | 1.00 | 43.71 | |
| ATOM | 1065 | N | LYS | 1598 | 23.621 | -15.881 | 21.544 | 1.00 | 40.61 | |
| ATOM | 1067 | CA | LYS | 1598 | 22.405 | -16.298 | 20.867 | 1.00 | 38.61 | |
| ATOM | 1068 | CB | LYS | 1598 | 21.848 | -17.575 | 21.483 | 1.00 | 36.33 | |
| ATOM | 1069 | CG | LYS | 1598 | 21.135 | -18.439 | 20.468 | 1.00 | 40.09 | |
| ATOM | 1070 | CD | LYS | 1598 | 20.213 | -19.434 | 21.118 | 1.00 | 43.39 | |
| ATOM | 1071 | CE | LYS | 1598 | 19.766 | -20.494 | 20.122 | 1.00 | 48.25 | |
| ATOM | 1072 | NZ | LYS | 1598 | 20.930 | -21.290 | 19.623 | 1.00 | 50.46 | |
| ATOM | 1076 | C | LYS | 1598 | 21.348 | -15.194 | 20.895 | 1.00 | 38.17 | |
| ATOM | 1077 | O | LYS | 1598 | 20.579 | -15.053 | 19.945 | 1.00 | 41.27 | |
| ATOM | 1078 | N | ASP | 1599 | 21.321 | -14.408 | 21.969 | 1.00 | 35.90 | |
| ATOM | 1080 | CA | ASP | 1599 | 20.366 | -13.307 | 22.099 | 1.00 | 34.08 | |
| ATOM | 1081 | CB | ASP | 1599 | 20.450 | -12.661 | 23.477 | 1.00 | 37.83 | |
| ATOM | 1082 | CG | ASP | 1599 | 19.822 | -13.505 | 24.562 | 1.00 | 39.93 | |
| ATOM | 1083 | OD1 | ASP | 1599 | 20.089 | -13.217 | 25.742 | 1.00 | 45.85 | |
| ATOM | 1084 | OD2 | ASP | 1599 | 19.060 | -14.444 | 24.240 | 1.00 | 41.06 | |
| ATOM | 1085 | C | ASP | 1599 | 20.634 | -12.243 | 21.061 | 1.00 | 32.37 | |
| ATOM | 1086 | O | ASP | 1599 | 19.704 | -11.701 | 20.466 | 1.00 | 32.58 | |
| ATOM | 1087 | N | LEU | 1600 | 21.915 | -11.945 | 20.873 | 1.00 | 30.45 | |
| ATOM | 1089 | CA | LEU | 1600 | 22.355 | -10.948 | 19.902 | 1.00 | 29.59 | |
| ATOM | 1090 | CB | LEU | 1600 | 23.841 | -10.654 | 20.097 | 1.00 | 28.59 | |
| ATOM | 1091 | CG | LEU | 1600 | 24.238 | -10.057 | 21.449 | 1.00 | 24.59 | |
| ATOM | 1092 | CD1 | LEU | 1600 | 25.747 | -9.869 | 21.522 | 1.00 | 18.40 | |
| ATOM | 1093 | CD2 | LEU | 1600 | 23.529 | -8.745 | 21.626 | 1.00 | 21.71 | |
| ATOM | 1094 | C | LEU | 1600 | 22.073 | -11.393 | 18.458 | 1.00 | 28.54 | |
| ATOM | 1095 | O | LEU | 1600 | 21.578 | -10.613 | 17.648 | 1.00 | 25.59 | |
| ATOM | 1096 | N | VAL | 1601 | 22.377 | -12.645 | 18.134 | 1.00 | 29.13 | |
| ATOM | 1098 | CA | VAL | 1601 | 22.111 | -13.154 | 16.793 | 1.00 | 29.74 | |
| ATOM | 1099 | CB | VAL | 1601 | 22.780 | -14.513 | 16.551 | 1.00 | 29.63 | |
| ATOM | 1100 | CG1 | VAL | 1601 | 22.615 | -14.922 | 15.105 | 1.00 | 29.30 | |
| ATOM | 1101 | CG2 | VAL | 1601 | 24.259 | -14.422 | 16.873 | 1.00 | 28.52 | |
| ATOM | 1102 | C | VAL | 1601 | 20.591 | -13.247 | 16.564 | 1.00 | 29.98 | |
| ATOM | 1103 | O | VAL | 1601 | 20.106 | -13.040 | 15.452 | 1.00 | 29.73 | |
| ATOM | 1104 | N | SER | 1602 | 19.855 | -13.493 | 17.645 | 1.00 | 30.97 | |
| ATOM | 1106 | CA | SER | 1602 | 18.399 | -13.576 | 17.607 | 1.00 | 29.64 | |
| ATOM | 1107 | CB | SER | 1602 | 17.894 | -14.141 | 18.925 | 1.00 | 30.45 | |
| ATOM | 1108 | OG | SER | 1602 | 16.483 | -14.158 | 18.962 | 1.00 | 39.63 | |
| ATOM | 1110 | C | SER | 1602 | 17.784 | -12.192 | 17.343 | 1.00 | 29.30 | |
| ATOM | 1111 | O | SER | 1602 | 16.772 | -12.071 | 16.641 | 1.00 | 28.74 | |
| ATOM | 1112 | N | CYS | 1603 | 18.385 | -11.157 | 17.925 | 1.00 | 27.68 | |
| ATOM | 1114 | CA | CYS | 1603 | 17.931 | -9.783 | 17.717 | 1.00 | 27.32 | |
| ATOM | 1115 | CB | CYS | 1603 | 18.791 | -8.790 | 18.516 | 1.00 | 25.40 | |
| ATOM | 1116 | SG | CYS | 1603 | 18.472 | -7.039 | 18.177 | 0.50 | 20.76 | PRT1 |
| ATOM | 1117 | C | CYS | 1603 | 18.057 | -9.468 | 16.225 | 1.00 | 28.34 | |
| ATOM | 1118 | O | CYS | 1603 | 17.134 | -8.926 | 15.629 | 1.00 | 29.70 | |
| ATOM | 1119 | N | ALA | 1604 | 19.192 | -9.837 | 15.627 | 1.00 | 29.36 | |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1121 | CA | ALA | 1604 | 19.438 | -9.601 | 14.195 | 1.00 | 28.78 |
| ATOM | 1122 | CB | ALA | 1604 | 20.861 | -10.066 | 13.808 | 1.00 | 22.61 |
| ATOM | 1123 | C | ALA | 1604 | 18.386 | -10.304 | 13.324 | 1.00 | 30.14 |
| ATOM | 1124 | O | ALA | 1604 | 17.792 | -9.690 | 12.426 | 1.00 | 31.64 |
| ATOM | 1125 | N | TYR | 1605 | 18.156 | -11.587 | 13.605 | 1.00 | 29.84 |
| ATOM | 1127 | CA | TYR | 1605 | 17.179 | -12.392 | 12.874 | 1.00 | 28.26 |
| ATOM | 1128 | CB | TYR | 1605 | 17.107 | -13.789 | 13.488 | 1.00 | 28.74 |
| ATOM | 1129 | CG | TYR | 1605 | 16.018 | -14.673 | 12.912 | 1.00 | 31.12 |
| ATOM | 1130 | CD1 | TYR | 1605 | 16.152 | -15.256 | 11.650 | 1.00 | 32.53 |
| ATOM | 1131 | CE1 | TYR | 1605 | 15.144 | -16.067 | 11.121 | 1.00 | 30.84 |
| ATOM | 1132 | CD2 | TYR | 1605 | 14.853 | -14.926 | 13.634 | 1.00 | 31.21 |
| ATOM | 1133 | CE2 | TYR | 1605 | 13.850 | -15.734 | 13.116 | 1.00 | 29.69 |
| ATOM | 1134 | CZ | TYR | 1605 | 14.002 | -16.296 | 11.864 | 1.00 | 30.82 |
| ATOM | 1135 | OH | TYR | 1605 | 12.990 | -17.069 | 11.359 | 1.00 | 33.77 |
| ATOM | 1137 | C | TYR | 1605 | 15.788 | -11.758 | 12.853 | 1.00 | 27.33 |
| ATOM | 1138 | O | TYR | 1605 | 15.152 | -11.691 | 11.805 | 1.00 | 27.94 |
| ATOM | 1139 | N | GLN | 1606 | 15.323 | -11.292 | 14.007 | 1.00 | 27.93 |
| ATOM | 1141 | CA | GLN | 1606 | 14.008 | -10.659 | 14.115 | 1.00 | 27.20 |
| ATOM | 1142 | CB | GLN | 1606 | 13.686 | -10.335 | 15.570 | 1.00 | 26.40 |
| ATOM | 1143 | CG | GLN | 1606 | 13.301 | -11.556 | 16.402 | 1.00 | 28.12 |
| ATOM | 1144 | CD | GLN | 1606 | 13.114 | -11.215 | 17.865 | 1.00 | 30.41 |
| ATOM | 1145 | OE1 | GLN | 1606 | 12.188 | -10.489 | 18.234 | 1.00 | 34.34 |
| ATOM | 1146 | NE2 | GLN | 1606 | 14.008 | -11.701 | 18.700 | 1.00 | 31.44 |
| ATOM | 1149 | C | GLN | 1606 | 13.906 | -9.397 | 13.275 | 1.00 | 29.67 |
| ATOM | 1150 | O | GLN | 1606 | 12.884 | -9.148 | 12.622 | 1.00 | 30.74 |
| ATOM | 1151 | N | VAL | 1607 | 14.970 | -8.602 | 13.281 | 1.00 | 29.59 |
| ATOM | 1153 | CA | VAL | 1607 | 14.996 | -7.377 | 12.501 | 1.00 | 27.00 |
| ATOM | 1154 | CB | VAL | 1607 | 16.235 | -6.544 | 12.842 | 1.00 | 27.20 |
| ATOM | 1155 | CG1 | VAL | 1607 | 16.382 | -5.397 | 11.859 | 1.00 | 28.11 |
| ATOM | 1156 | CG2 | VAL | 1607 | 16.113 | -5.996 | 14.266 | 1.00 | 24.79 |
| ATOM | 1157 | C | VAL | 1607 | 14.966 | -7.725 | 11.014 | 1.00 | 28.02 |
| ATOM | 1158 | O | VAL | 1607 | 14.229 | -7.108 | 10.241 | 1.00 | 28.28 |
| ATOM | 1159 | N | ALA | 1608 | 15.736 | -8.741 | 10.626 | 1.00 | 27.56 |
| ATOM | 1161 | CA | ALA | 1608 | 15.787 | -9.206 | 9.236 | 1.00 | 27.36 |
| ATOM | 1162 | CB | ALA | 1608 | 16.801 | -10.339 | 9.095 | 1.00 | 26.25 |
| ATOM | 1163 | C | ALA | 1608 | 14.402 | -9.674 | 8.779 | 1.00 | 28.58 |
| ATOM | 1164 | O | ALA | 1608 | 14.013 | -9.446 | 7.624 | 1.00 | 29.11 |
| ATOM | 1165 | N | ARG | 1609 | 13.660 | -10.326 | 9.680 | 1.00 | 28.88 |
| ATOM | 1167 | CA | ARG | 1609 | 12.306 | -10.797 | 9.376 | 1.00 | 27.17 |
| ATOM | 1168 | CB | ARG | 1609 | 11.797 | -11.731 | 10.464 | 1.00 | 29.68 |
| ATOM | 1169 | CG | ARG | 1609 | 12.458 | -13.062 | 10.439 | 1.00 | 31.65 |
| ATOM | 1170 | CD | ARG | 1609 | 11.612 | -14.049 | 11.177 | 1.00 | 38.21 |
| ATOM | 1171 | NE | ARG | 1609 | 10.856 | -14.897 | 10.269 | 1.00 | 41.10 |
| ATOM | 1173 | CZ | ARG | 1609 | 10.048 | -15.872 | 10.667 | 1.00 | 41.97 |
| ATOM | 1174 | NH1 | ARG | 1609 | 9.886 | -16.125 | 11.959 | 1.00 | 40.69 |
| ATOM | 1177 | NH2 | ARG | 1609 | 9.411 | -16.609 | 9.770 | 1.00 | 43.57 |
| ATOM | 1180 | C | ARG | 1609 | 11.312 | -9.654 | 9.183 | 1.00 | 25.38 |
| ATOM | 1181 | O | ARG | 1609 | 10.480 | -9.693 | 8.260 | 1.00 | 25.75 |
| ATOM | 1182 | N | GLY | 1610 | 11.365 | -8.661 | 10.070 | 1.00 | 24.03 |
| ATOM | 1184 | CA | GLY | 1610 | 10.480 | -7.517 | 9.939 | 1.00 | 21.74 |
| ATOM | 1185 | C | GLY | 1610 | 10.734 | -6.864 | 8.592 | 1.00 | 23.32 |
| ATOM | 1186 | O | GLY | 1610 | 9.805 | -6.540 | 7.850 | 1.00 | 23.39 |
| ATOM | 1187 | N | MET | 1611 | 12.016 | -6.714 | 8.265 | 1.00 | 24.48 |
| ATOM | 1189 | CA | MET | 1611 | 12.453 | -6.125 | 7.002 | 1.00 | 23.13 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1190 | CB | MET | 1611 | 13.949 | -5.860 | 7.035 | 1.00 | 19.46 |
| ATOM | 1191 | CG | MET | 1611 | 14.339 | -4.671 | 7.910 | 1.00 | 22.46 |
| ATOM | 1192 | SD | MET | 1611 | 13.457 | -3.123 | 7.536 | 1.00 | 25.27 |
| ATOM | 1193 | CE | MET | 1611 | 13.900 | -2.801 | 5.876 | 1.00 | 22.25 |
| ATOM | 1194 | C | MET | 1611 | 12.100 | -7.005 | 5.811 | 1.00 | 24.87 |
| ATOM | 1195 | O | MET | 1611 | 11.699 | -6.497 | 4.755 | 1.00 | 24.09 |
| ATOM | 1196 | N | GLU | 1612 | 12.230 | -8.321 | 5.975 | 1.00 | 25.48 |
| ATOM | 1198 | CA | GLU | 1612 | 11.894 | -9.232 | 4.890 | 1.00 | 25.42 |
| ATOM | 1199 | CB | GLU | 1612 | 12.155 | -10.691 | 5.288 | 1.00 | 23.41 |
| ATOM | 1200 | CG | GLU | 1612 | 11.664 | -11.679 | 4.232 | 1.00 | 25.14 |
| ATOM | 1201 | CD | GLU | 1612 | 11.872 | -13.141 | 4.599 | 1.00 | 28.60 |
| ATOM | 1202 | OE1 | GLU | 1612 | 11.637 | -13.514 | 5.777 | 1.00 | 30.10 |
| ATOM | 1203 | OE2 | GLU | 1612 | 12.244 | -13.928 | 3.694 | 1.00 | 29.53 |
| ATOM | 1204 | C | GLU | 1612 | 10.418 | -9.021 | 4.521 | 1.00 | 26.92 |
| ATOM | 1205 | O | GLU | 1612 | 10.065 | -8.928 | 3.343 | 1.00 | 29.61 |
| ATOM | 1206 | N | TYR | 1613 | 9.576 | -8.884 | 5.542 | 1.00 | 27.88 |
| ATOM | 1208 | CA | TYR | 1613 | 8.154 | -8.675 | 5.337 | 1.00 | 23.82 |
| ATOM | 1209 | CB | TYR | 1613 | 7.415 | -8.769 | 6.667 | 1.00 | 24.17 |
| ATOM | 1210 | CG | TYR | 1613 | 5.941 | -8.492 | 6.545 | 1.00 | 23.73 |
| ATOM | 1211 | CD1 | TYR | 1613 | 5.064 | -9.483 | 6.096 | 1.00 | 22.17 |
| ATOM | 1212 | CE1 | TYR | 1613 | 3.698 | -9.235 | 5.965 | 1.00 | 21.08 |
| ATOM | 1213 | CD2 | TYR | 1613 | 5.419 | -7.237 | 6.865 | 1.00 | 23.16 |
| ATOM | 1214 | CE2 | TYR | 1613 | 4.054 | -6.976 | 6.736 | 1.00 | 26.38 |
| ATOM | 1215 | CZ | TYR | 1613 | 3.200 | -7.981 | 6.287 | 1.00 | 23.16 |
| ATOM | 1216 | OH | TYR | 1613 | 1.855 | -7.725 | 6.149 | 1.00 | 25.50 |
| ATOM | 1218 | C | TYR | 1613 | 7.885 | -7.327 | 4.670 | 1.00 | 23.17 |
| ATOM | 1219 | O | TYR | 1613 | 7.147 | -7.246 | 3.689 | 1.00 | 24.21 |
| ATOM | 1220 | N | LEU | 1614 | 8.481 | -6.266 | 5.206 | 1.00 | 23.04 |
| ATOM | 1222 | CA | LEU | 1614 | 8.316 | -4.920 | 4.652 | 1.00 | 21.81 |
| ATOM | 1223 | CB | LEU | 1614 | 9.107 | -3.906 | 5.484 | 1.00 | 19.94 |
| ATOM | 1224 | CG | LEU | 1614 | 8.609 | -3.616 | 6.902 | 1.00 | 21.94 |
| ATOM | 1225 | CD1 | LEU | 1614 | 9.580 | -2.719 | 7.654 | 1.00 | 14.28 |
| ATOM | 1226 | CD2 | LEU | 1614 | 7.227 | -2.977 | 6.814 | 1.00 | 17.45 |
| ATOM | 1227 | C | LEU | 1614 | 8.764 | -4.858 | 3.182 | 1.00 | 23.74 |
| ATOM | 1228 | O | LEU | 1614 | 8.169 | -4.150 | 2.367 | 1.00 | 25.26 |
| ATOM | 1229 | N | ALA | 1615 | 9.831 | -5.587 | 2.862 | 1.00 | 25.00 |
| ATOM | 1231 | CA | ALA | 1615 | 10.357 | -5.644 | 1.502 | 1.00 | 23.04 |
| ATOM | 1232 | CB | ALA | 1615 | 11.710 | -6.360 | 1.483 | 1.00 | 20.02 |
| ATOM | 1233 | C | ALA | 1615 | 9.351 | -6.357 | 0.605 | 1.00 | 23.15 |
| ATOM | 1234 | O | ALA | 1615 | 9.076 | -5.891 | -0.503 | 1.00 | 25.25 |
| ATOM | 1235 | N | SER | 1616 | 8.754 | -7.441 | 1.104 | 1.00 | 23.64 |
| ATOM | 1237 | CA | SER | 1616 | 7.758 | -8.199 | 0.337 | 1.00 | 23.60 |
| ATOM | 1238 | CB | SER | 1616 | 7.346 | -9.453 | 1.107 | 1.00 | 22.46 |
| ATOM | 1239 | OG | SER | 1616 | 6.531 | -9.131 | 2.224 | 1.00 | 26.66 |
| ATOM | 1241 | C | SER | 1616 | 6.505 | -7.369 | 0.025 | 1.00 | 25.45 |
| ATOM | 1242 | O | SER | 1616 | 5.813 | -7.607 | -0.967 | 1.00 | 26.67 |
| ATOM | 1243 | N | LYS | 1617 | 6.193 | -6.436 | 0.916 | 1.00 | 25.47 |
| ATOM | 1245 | CA | LYS | 1617 | 5.051 | -5.551 | 0.781 | 1.00 | 25.04 |
| ATOM | 1246 | CB | LYS | 1617 | 4.513 | -5.183 | 2.163 | 1.00 | 26.30 |
| ATOM | 1247 | CG | LYS | 1617 | 3.778 | -6.318 | 2.851 | 1.00 | 28.58 |
| ATOM | 1248 | CD | LYS | 1617 | 2.438 | -6.530 | 2.169 | 1.00 | 33.00 |
| ATOM | 1249 | CE | LYS | 1617 | 1.652 | -7.676 | 2.764 | 1.00 | 38.57 |
| ATOM | 1250 | NZ | LYS | 1617 | 2.167 | -8.987 | 2.300 | 1.00 | 45.15 |
| ATOM | 1254 | C | LYS | 1617 | 5.417 | -4.293 | 0.002 | 1.00 | 26.34 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1255 | O | LYS | 1617 | 4.649 | -3.336 | -0.034 | 1.00 | 26.77 |
| ATOM | 1256 | N | LYS | 1618 | 6.592 | -4.319 | -0.632 | 1.00 | 27.17 |
| ATOM | 1258 | CA | LYS | 1618 | 7.084 | -3.197 | -1.447 | 1.00 | 28.20 |
| ATOM | 1259 | CB | LYS | 1618 | 6.053 | -2.819 | -2.528 | 1.00 | 28.42 |
| ATOM | 1260 | CG | LYS | 1618 | 5.971 | -3.749 | -3.730 | 1.00 | 26.63 |
| ATOM | 1261 | CD | LYS | 1618 | 5.573 | -5.163 | -3.364 | 1.00 | 30.45 |
| ATOM | 1262 | CE | LYS | 1618 | 5.636 | -6.087 | -4.570 | 1.00 | 32.50 |
| ATOM | 1263 | NZ | LYS | 1618 | 4.621 | -5.729 | -5.600 | 1.00 | 34.89 |
| ATOM | 1267 | C | LYS | 1618 | 7.466 | -1.951 | -0.643 | 1.00 | 28.78 |
| ATOM | 1268 | O | LYS | 1618 | 7.556 | -0.848 | -1.199 | 1.00 | 28.78 |
| ATOM | 1269 | N | CYS | 1619 | 7.753 | -2.130 | 0.646 | 1.00 | 29.26 |
| ATOM | 1271 | CA | CYS | 1619 | 8.111 | -1.022 | 1.522 | 1.00 | 28.32 |
| ATOM | 1272 | CB | CYS | 1619 | 7.391 | -1.173 | 2.873 | 1.00 | 26.33 |
| ATOM | 1273 | SG | CYS | 1619 | 7.754 | 0.105 | 4.136 | 1.00 | 27.82 |
| ATOM | 1274 | C | CYS | 1619 | 9.622 | -0.841 | 1.728 | 1.00 | 29.15 |
| ATOM | 1275 | O | CYS | 1619 | 10.336 | -1.786 | 2.072 | 1.00 | 29.55 |
| ATOM | 1276 | N | ILE | 1620 | 10.096 | 0.378 | 1.457 | 1.00 | 29.39 |
| ATOM | 1278 | CA | ILE | 1620 | 11.502 | 0.761 | 1.625 | 1.00 | 27.44 |
| ATOM | 1279 | CB | ILE | 1620 | 12.030 | 1.543 | 0.381 | 1.00 | 25.37 |
| ATOM | 1280 | CG2 | ILE | 1620 | 13.521 | 1.806 | 0.506 | 1.00 | 19.80 |
| ATOM | 1281 | CG1 | ILE | 1620 | 11.767 | 0.764 | -0.913 | 1.00 | 25.40 |
| ATOM | 1282 | CD1 | ILE | 1620 | 12.100 | 1.557 | -2.164 | 1.00 | 27.51 |
| ATOM | 1283 | C | ILE | 1620 | 11.553 | 1.686 | 2.855 | 1.00 | 26.56 |
| ATOM | 1284 | O | ILE | 1620 | 11.011 | 2.792 | 2.833 | 1.00 | 26.68 |
| ATOM | 1285 | N | HIS | 1621 | 12.193 | 1.210 | 3.916 | 1.00 | 26.31 |
| ATOM | 1287 | CA | HIS | 1621 | 12.297 | 1.967 | 5.162 | 1.00 | 25.00 |
| ATOM | 1288 | CB | HIS | 1621 | 13.081 | 1.174 | 6.210 | 1.00 | 23.08 |
| ATOM | 1289 | CG | HIS | 1621 | 12.848 | 1.633 | 7.618 | 1.00 | 23.21 |
| ATOM | 1290 | CD2 | HIS | 1621 | 12.224 | 1.027 | 8.656 | 1.00 | 22.69 |
| ATOM | 1291 | ND1 | HIS | 1621 | 13.260 | 2.862 | 8.088 | 1.00 | 25.34 |
| ATOM | 1293 | CE1 | HIS | 1621 | 12.909 | 2.993 | 9.356 | 1.00 | 24.18 |
| ATOM | 1294 | NE2 | HIS | 1621 | 12.273 | 1.891 | 9.719 | 1.00 | 25.86 |
| ATOM | 1296 | C | HIS | 1621 | 12.963 | 3.316 | 4.976 | 1.00 | 25.09 |
| ATOM | 1297 | O | HIS | 1621 | 12.408 | 4.328 | 5.349 | 1.00 | 28.21 |
| ATOM | 1298 | N | ARG | 1622 | 14.162 | 3.315 | 4.402 | 1.00 | 26.09 |
| ATOM | 1300 | CA | ARG | 1622 | 14.976 | 4.520 | 4.183 | 1.00 | 26.50 |
| ATOM | 1301 | CB | ARG | 1622 | 14.180 | 5.670 | 3.558 | 1.00 | 23.52 |
| ATOM | 1302 | CG | ARG | 1622 | 13.673 | 5.326 | 2.202 | 1.00 | 23.81 |
| ATOM | 1303 | CD | ARG | 1622 | 12.995 | 6.494 | 1.551 | 1.00 | 28.42 |
| ATOM | 1304 | NE | ARG | 1622 | 12.677 | 6.170 | 0.180 | 1.00 | 32.52 |
| ATOM | 1306 | CZ | ARG | 1622 | 11.623 | 5.455 | -0.197 | 1.00 | 32.34 |
| ATOM | 1307 | NH1 | ARG | 1622 | 10.774 | 4.994 | 0.711 | 1.00 | 30.07 |
| ATOM | 1310 | NH2 | ARG | 1622 | 11.460 | 5.138 | -1.489 | 1.00 | 28.30 |
| ATOM | 1313 | C | ARG | 1622 | 15.740 | 4.993 | 5.423 | 1.00 | 26.31 |
| ATOM | 1314 | O | ARG | 1622 | 16.698 | 5.757 | 5.313 | 1.00 | 26.19 |
| ATOM | 1315 | N | ASP | 1623 | 15.379 | 4.495 | 6.596 | 1.00 | 27.41 |
| ATOM | 1317 | CA | ASP | 1623 | 16.114 | 4.879 | 7.788 | 1.00 | 29.94 |
| ATOM | 1318 | CB | ASP | 1623 | 15.562 | 6.155 | 8.430 | 1.00 | 34.83 |
| ATOM | 1319 | CG | ASP | 1623 | 16.481 | 6.689 | 9.533 | 1.00 | 38.84 |
| ATOM | 1320 | OD1 | ASP | 1623 | 15.971 | 7.265 | 10.514 | 1.00 | 44.51 |
| ATOM | 1321 | OD2 | ASP | 1623 | 17.721 | 6.514 | 9.423 | 1.00 | 37.59 |
| ATOM | 1322 | C | ASP | 1623 | 16.203 | 3.763 | 8.812 | 1.00 | 28.71 |
| ATOM | 1323 | O | ASP | 1623 | 15.845 | 3.927 | 9.990 | 1.00 | 26.21 |
| ATOM | 1324 | N | LEU | 1624 | 16.735 | 2.633 | 8.357 | 1.00 | 26.82 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1326 | CA | LEU | 1624 | 16.905 | 1.469 | 9.216 | 1.00 | 25.91 |
| ATOM | 1327 | CB | LEU | 1624 | 17.025 | 0.209 | 8.367 | 1.00 | 23.35 |
| ATOM | 1328 | CG | LEU | 1624 | 17.089 | -1.107 | 9.127 | 1.00 | 21.09 |
| ATOM | 1329 | CD1 | LEU | 1624 | 15.824 | -1.303 | 10.009 | 1.00 | 14.44 |
| ATOM | 1330 | CD2 | LEU | 1624 | 17.282 | -2.215 | 8.101 | 1.00 | 18.30 |
| ATOM | 1331 | C | LEU | 1624 | 18.136 | 1.640 | 10.105 | 1.00 | 24.93 |
| ATOM | 1332 | O | LEU | 1624 | 19.235 | 1.897 | 9.611 | 1.00 | 25.58 |
| ATOM | 1333 | N | ALA | 1625 | 17.912 | 1.557 | 11.416 | 1.00 | 26.30 |
| ATOM | 1335 | CA | ALA | 1625 | 18.945 | 1.702 | 12.445 | 1.00 | 23.59 |
| ATOM | 1336 | CB | ALA | 1625 | 19.271 | 3.174 | 12.654 | 1.00 | 15.82 |
| ATOM | 1337 | C | ALA | 1625 | 18.351 | 1.116 | 13.732 | 1.00 | 23.64 |
| ATOM | 1338 | O | ALA | 1625 | 17.135 | 0.928 | 13.825 | 1.00 | 26.66 |
| ATOM | 1339 | N | ALA | 1626 | 19.197 | 0.815 | 14.712 | 1.00 | 21.59 |
| ATOM | 1341 | CA | ALA | 1626 | 18.708 | 0.266 | 15.974 | 1.00 | 21.66 |
| ATOM | 1342 | CB | ALA | 1626 | 19.860 | -0.179 | 16.838 | 1.00 | 22.97 |
| ATOM | 1343 | C | ALA | 1626 | 17.835 | 1.272 | 16.731 | 1.00 | 24.98 |
| ATOM | 1344 | O | ALA | 1626 | 17.072 | 0.891 | 17.620 | 1.00 | 26.84 |
| ATOM | 1345 | N | ARG | 1627 | 17.978 | 2.558 | 16.409 | 1.00 | 24.55 |
| ATOM | 1347 | CA | ARG | 1627 | 17.178 | 3.598 | 17.042 | 1.00 | 25.29 |
| ATOM | 1348 | CB | ARG | 1627 | 17.699 | 4.983 | 16.673 | 1.00 | 26.66 |
| ATOM | 1349 | CG | ARG | 1627 | 17.675 | 5.276 | 15.179 | 1.00 | 30.56 |
| ATOM | 1350 | CD | ARG | 1627 | 18.033 | 6.715 | 14.902 | 1.00 | 34.97 |
| ATOM | 1351 | NE | ARG | 1627 | 18.177 | 6.980 | 13.470 | 1.00 | 40.03 |
| ATOM | 1353 | CZ | ARG | 1627 | 19.322 | 6.864 | 12.809 | 1.00 | 40.62 |
| ATOM | 1354 | NH1 | ARG | 1627 | 20.421 | 6.485 | 13.441 | 1.00 | 46.52 |
| ATOM | 1357 | NH2 | ARG | 1627 | 19.377 | 7.159 | 11.523 | 1.00 | 43.25 |
| ATOM | 1360 | C | ARG | 1627 | 15.739 | | | | |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1394 | CG1 | VAL | 1631 | 12.995 | -5.469 | 23.243 | 1.00 | 23.92 |
| ATOM | 1395 | CG2 | VAL | 1631 | 14.197 | -3.714 | 21.895 | 1.00 | 24.26 |
| ATOM | 1396 | C | VAL | 1631 | 10.450 | -3.773 | 22.885 | 1.00 | 32.64 |
| ATOM | 1397 | O | VAL | 1631 | 10.198 | -2.821 | 23.643 | 1.00 | 33.01 |
| ATOM | 1398 | N | THR | 1632 | 9.697 | -4.863 | 22.827 | 1.00 | 34.45 |
| ATOM | 1400 | CA | THR | 1632 | 8.516 | -5.035 | 23.660 | 1.00 | 34.29 |
| ATOM | 1401 | CB | THR | 1632 | 7.466 | -5.941 | 22.962 | 1.00 | 34.62 |
| ATOM | 1402 | OG1 | THR | 1632 | 7.965 | -7.288 | 22.881 | 1.00 | 34.40 |
| ATOM | 1404 | CG2 | THR | 1632 | 7.154 | -5.414 | 21.551 | 1.00 | 31.61 |
| ATOM | 1405 | C | THR | 1632 | 8.896 | -5.678 | 24.989 | 1.00 | 35.41 |
| ATOM | 1406 | O | THR | 1632 | 10.002 | -6.189 | 25.146 | 1.00 | 34.79 |
| ATOM | 1407 | N | GLU | 1633 | 7.939 | -5.706 | 25.913 | 1.00 | 36.86 |
| ATOM | 1409 | CA | GLU | 1633 | 8.156 | -6.298 | 27.224 | 1.00 | 37.27 |
| ATOM | 1410 | CB | GLU | 1633 | 6.893 | -6.182 | 28.079 | 1.00 | 37.66 |
| ATOM | 1411 | CG | GLU | 1633 | 7.031 | -6.718 | 29.514 | 1.00 | 44.43 |
| ATOM | 1412 | CD | GLU | 1633 | 8.048 | -5.959 | 30.378 | 1.00 | 46.68 |
| ATOM | 1413 | OE1 | GLU | 1633 | 8.104 | -4.708 | 30.300 | 1.00 | 49.88 |
| ATOM | 1414 | OE2 | GLU | 1633 | 8.783 | -6.612 | 31.156 | 1.00 | 48.53 |
| ATOM | 1415 | C | GLU | 1633 | 8.561 | -7.753 | 27.088 | 1.00 | 37.15 |
| ATOM | 1416 | O | GLU | 1633 | 9.227 | -8.292 | 27.954 | 1.00 | 38.60 |
| ATOM | 1417 | N | ASP | 1634 | 8.167 | -8.384 | 25.990 | 1.00 | 38.41 |
| ATOM | 1419 | CA | ASP | 1634 | 8.505 | -9.787 | 25.770 | 1.00 | 38.86 |
| ATOM | 1420 | CB | ASP | 1634 | 7.381 | -10.499 | 25.013 | 1.00 | 44.27 |
| ATOM | 1421 | CG | ASP | 1634 | 6.022 | -10.349 | 25.690 | 1.00 | 50.18 |
| ATOM | 1422 | OD1 | ASP | 1634 | 5.726 | -11.141 | 26.617 | 1.00 | 52.07 |
| ATOM | 1423 | OD2 | ASP | 1634 | 5.253 | -9.439 | 25.295 | 1.00 | 50.17 |
| ATOM | 1424 | C | ASP | 1634 | 9.804 | -9.947 | 25.007 | 1.00 | 36.23 |
| ATOM | 1425 | O | ASP | 1634 | 10.141 | -11.049 | 24.608 | 1.00 | 35.82 |
| ATOM | 1426 | N | ASN | 1635 | 10.528 | -8.851 | 24.799 | 1.00 | 36.51 |
| ATOM | 1428 | CA | ASN | 1635 | 11.795 | -8.864 | 24.052 | 1.00 | 37.41 |
| ATOM | 1429 | CB | ASN | 1635 | 12.801 | -9.842 | 24.678 | 1.00 | 38.49 |
| ATOM | 1430 | CG | ASN | 1635 | 13.343 | -9.359 | 26.003 | 1.00 | 37.71 |
| ATOM | 1431 | OD1 | ASN | 1635 | 13.499 | -8.156 | 26.227 | 1.00 | 38.09 |
| ATOM | 1432 | ND2 | ASN | 1635 | 13.679 | -10.300 | 26.874 | 1.00 | 39.63 |
| ATOM | 1435 | C | ASN | 1635 | 11.655 | -9.162 | 22.552 | 1.00 | 36.37 |
| ATOM | 1436 | O | ASN | 1635 | 12.522 | -9.811 | 21.944 | 1.00 | 36.41 |
| ATOM | 1437 | N | VAL | 1636 | 10.547 | -8.721 | 21.966 | 1.00 | 33.79 |
| ATOM | 1439 | CA | VAL | 1636 | 10.315 | -8.910 | 20.543 | 1.00 | 30.59 |
| ATOM | 1440 | CB | VAL | 1636 | 8.820 | -9.139 | 20.218 | 1.00 | 28.83 |
| ATOM | 1441 | CG1 | VAL | 1636 | 8.615 | -9.182 | 18.712 | 1.00 | 26.13 |
| ATOM | 1442 | CG2 | VAL | 1636 | 8.339 | -10.431 | 20.838 | 1.00 | 25.67 |
| ATOM | 1443 | C | VAL | 1636 | 10.782 | -7.630 | 19.863 | 1.00 | 30.18 |
| ATOM | 1444 | O | VAL | 1636 | 10.436 | -6.527 | 20.301 | 1.00 | 27.86 |
| ATOM | 1445 | N | MET | 1637 | 11.609 | -7.792 | 18.832 | 1.00 | 30.93 |
| ATOM | 1447 | CA | MET | 1637 | 12.140 | -6.679 | 18.060 | 1.00 | 28.34 |
| ATOM | 1448 | CB | MET | 1637 | 13.397 | -7.138 | 17.330 | 1.00 | 30.84 |
| ATOM | 1449 | CG | MET | 1637 | 14.480 | -7.693 | 18.254 | 1.00 | 30.73 |
| ATOM | 1450 | SD | MET | 1637 | 15.050 | -6.490 | 19.477 | 1.00 | 32.20 |
| ATOM | 1451 | CE | MET | 1637 | 15.074 | -7.500 | 20.938 | 1.00 | 28.71 |
| ATOM | 1452 | C | MET | 1637 | 11.082 | -6.264 | 17.051 | 1.00 | 27.29 |
| ATOM | 1453 | O | MET | 1637 | 10.587 | -7.099 | 16.297 | 1.00 | 27.32 |
| ATOM | 1454 | N | LYS | 1638 | 10.733 | -4.983 | 17.045 | 1.00 | 27.19 |
| ATOM | 1456 | CA | LYS | 1638 | 9.716 | -4.450 | 16.143 | 1.00 | 26.38 |
| ATOM | 1457 | CB | LYS | 1638 | 8.437 | -4.120 | 16.912 | 1.00 | 27.09 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1458 | CG | LYS | 1638 | 7.702 | -5.351 | 17.407 | 1.00 | 29.71 |
| ATOM | 1459 | CD | LYS | 1638 | 6.386 | -5.018 | 18.109 | 1.00 | 31.48 |
| ATOM | 1460 | CE | LYS | 1638 | 5.485 | -6.263 | 18.202 | 1.00 | 27.09 |
| ATOM | 1461 | NZ | LYS | 1638 | 4.888 | -6.561 | 16.869 | 1.00 | 26.68 |
| ATOM | 1465 | C | LYS | 1638 | 10.196 | -3.208 | 15.416 | 1.00 | 26.56 |
| ATOM | 1466 | O | LYS | 1638 | 10.514 | -2.194 | 16.040 | 1.00 | 27.40 |
| ATOM | 1467 | N | ILE | 1639 | 10.211 | -3.271 | 14.092 | 1.00 | 24.31 |
| ATOM | 1469 | CA | ILE | 1639 | 10.649 | -2.147 | 13.289 | 1.00 | 24.84 |
| ATOM | 1470 | CB | ILE | 1639 | 10.924 | -2.588 | 11.836 | 1.00 | 25.81 |
| ATOM | 1471 | CG2 | ILE | 1639 | 11.248 | -1.395 | 10.952 | 1.00 | 24.18 |
| ATOM | 1472 | CG1 | ILE | 1639 | 12.094 | -3.566 | 11.826 | 1.00 | 25.01 |
| ATOM | 1473 | CD1 | ILE | 1639 | 12.075 | -4.499 | 10.675 | 1.00 | 27.90 |
| ATOM | 1474 | C | ILE | 1639 | 9.641 | -0.999 | 13.348 | 1.00 | 24.90 |
| ATOM | 1475 | O | ILE | 1639 | 8.435 | -1.186 | 13.170 | 1.00 | 25.24 |
| ATOM | 1476 | N | ALA | 1640 | 10.167 | 0.183 | 13.635 | 1.00 | 25.70 |
| ATOM | 1478 | CA | ALA | 1640 | 9.378 | 1.392 | 13.744 | 1.00 | 27.61 |
| ATOM | 1479 | CB | ALA | 1640 | 9.699 | 2.094 | 15.070 | 1.00 | 26.37 |
| ATOM | 1480 | C | ALA | 1640 | 9.637 | 2.348 | 12.576 | 1.00 | 28.35 |
| ATOM | 1481 | O | ALA | 1640 | 10.650 | 2.243 | 11.871 | 1.00 | 28.40 |
| ATOM | 1482 | N | ASP | 1641 | 8.676 | 3.237 | 12.354 | 1.00 | 29.74 |
| ATOM | 1484 | CA | ASP | 1641 | 8.760 | 4.272 | 11.325 | 1.00 | 32.13 |
| ATOM | 1485 | CB | ASP | 1641 | 9.873 | 5.273 | 11.688 | 1.00 | 34.31 |
| ATOM | 1486 | CG | ASP | 1641 | 9.507 | 6.158 | 12.896 | 1.00 | 36.31 |
| ATOM | 1487 | OD1 | ASP | 1641 | 10.299 | 7.056 | 13.258 | 1.00 | 42.18 |
| ATOM | 1488 | OD2 | ASP | 1641 | 8.420 | 5.974 | 13.483 | 1.00 | 41.03 |
| ATOM | 1489 | C | ASP | 1641 | 8.882 | 3.840 | 9.867 | 1.00 | 32.00 |
| ATOM | 1490 | O | ASP | 1641 | 9.339 | 4.617 | 9.021 | 1.00 | 32.65 |
| ATOM | 1491 | N | PHE | 1642 | 8.415 | 2.634 | 9.563 | 1.00 | 30.61 |
| ATOM | 1493 | CA | PHE | 1642 | 8.473 | 2.119 | 8.200 | 1.00 | 30.06 |
| ATOM | 1494 | CB | PHE | 1642 | 8.248 | 0.606 | 8.189 | 1.00 | 24.46 |
| ATOM | 1495 | CG | PHE | 1642 | 6.981 | 0.176 | 8.854 | 1.00 | 23.26 |
| ATOM | 1496 | CD1 | PHE | 1642 | 5.799 | 0.075 | 8.125 | 1.00 | 19.66 |
| ATOM | 1497 | CD2 | PHE | 1642 | 6.966 | -0.134 | 10.209 | 1.00 | 22.88 |
| ATOM | 1498 | CE1 | PHE | 1642 | 4.609 | -0.331 | 8.734 | 1.00 | 20.97 |
| ATOM | 1499 | CE2 | PHE | 1642 | 5.785 | -0.540 | 10.830 | 1.00 | 26.61 |
| ATOM | 1500 | CZ | PHE | 1642 | 4.599 | -0.639 | 10.083 | 1.00 | 24.82 |
| ATOM | 1501 | C | PHE | 1642 | 7.512 | 2.830 | 7.225 | 1.00 | 33.14 |
| ATOM | 1502 | O | PHE | 1642 | 7.791 | 2.922 | 6.029 | 1.00 | 36.48 |
| ATOM | 1503 | N | GLY | 1643 | 6.411 | 3.372 | 7.741 | 1.00 | 32.65 |
| ATOM | 1505 | CA | GLY | 1643 | 5.462 | 4.059 | 6.876 | 1.00 | 32.28 |
| ATOM | 1506 | C | GLY | 1643 | 5.629 | 5.560 | 6.913 | 1.00 | 32.19 |
| ATOM | 1507 | O | GLY | 1643 | 4.795 | 6.310 | 6.415 | 1.00 | 30.74 |
| ATOM | 1508 | N | LEU | 1644 | 6.739 | 5.997 | 7.486 | 1.00 | 36.80 |
| ATOM | 1510 | CA | LEU | 1644 | 7.052 | 7.406 | 7.630 | 1.00 | 41.95 |
| ATOM | 1511 | CB | LEU | 1644 | 8.332 | 7.551 | 8.439 | 1.00 | 37.41 |
| ATOM | 1512 | CG | LEU | 1644 | 8.377 | 8.746 | 9.369 | 1.00 | 38.98 |
| ATOM | 1513 | CD1 | LEU | 1644 | 7.384 | 8.548 | 10.493 | 1.00 | 40.45 |
| ATOM | 1514 | CD2 | LEU | 1644 | 9.775 | 8.904 | 9.929 | 1.00 | 41.94 |
| ATOM | 1515 | C | LEU | 1644 | 7.189 | 8.150 | 6.296 | 1.00 | 47.55 |
| ATOM | 1516 | O | LEU | 1644 | 7.787 | 7.648 | 5.341 | 1.00 | 50.55 |
| ATOM | 1517 | N | ALA | 1645 | 6.637 | 9.356 | 6.247 | 1.00 | 52.59 |
| ATOM | 1519 | CA | ALA | 1645 | 6.686 | 10.194 | 5.055 | 1.00 | 56.88 |
| ATOM | 1520 | CB | ALA | 1645 | 5.391 | 10.999 | 4.942 | 1.00 | 58.01 |
| ATOM | 1521 | C | ALA | 1645 | 7.880 | 11.135 | 5.178 | 1.00 | 58.95 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1522 | O | ALA | 1645 | 8.064 | 11.770 | 6.224 | 1.00 | 59.37 |
| ATOM | 1523 | N | ARG | 1646 | 8.700 | 11.211 | 4.133 | 1.00 | 60.26 |
| ATOM | 1525 | CA | ARG | 1646 | 9.870 | 12.088 | 4.165 | 1.00 | 63.04 |
| ATOM | 1526 | CB | ARG | 1646 | 10.995 | 11.444 | 4.976 | 1.00 | 64.92 |
| ATOM | 1527 | C | ARG | 1646 | 10.377 | 12.461 | 2.782 | 1.00 | 63.84 |
| ATOM | 1528 | O | ARG | 1646 | 10.361 | 11.641 | 1.864 | 1.00 | 63.55 |
| ATOM | 1529 | N | ASP | 1647 | 10.801 | 13.714 | 2.633 | 1.00 | 65.18 |
| ATOM | 1531 | CA | ASP | 1647 | 11.332 | 14.190 | 1.361 | 1.00 | 67.26 |
| ATOM | 1532 | CB | ASP | 1647 | 10.989 | 15.670 | 1.150 | 1.00 | 68.92 |
| ATOM | 1533 | CG | ASP | 1647 | 11.164 | 16.124 | -0.304 | 1.00 | 70.88 |
| ATOM | 1534 | OD1 | ASP | 1647 | 12.196 | 15.811 | -0.943 | 1.00 | 70.33 |
| ATOM | 1535 | OD2 | ASP | 1647 | 10.258 | 16.825 | -0.808 | 1.00 | 71.39 |
| ATOM | 1536 | C | ASP | 1647 | 12.847 | 14.005 | 1.405 | 1.00 | 68.40 |
| ATOM | 1537 | O | ASP | 1647 | 13.545 | 14.711 | 2.142 | 1.00 | 68.66 |
| ATOM | 1538 | N | ILE | 1648 | 13.347 | 13.055 | 0.621 | 1.00 | 68.48 |
| ATOM | 1540 | CA | ILE | 1648 | 14.777 | 12.773 | 0.570 | 1.00 | 69.00 |
| ATOM | 1541 | CB | ILE | 1648 | 15.091 | 11.535 | -0.314 | 1.00 | 66.28 |
| ATOM | 1542 | CG2 | ILE | 1648 | 14.231 | 10.352 | 0.131 | 1.00 | 65.14 |
| ATOM | 1543 | CG1 | ILE | 1648 | 14.869 | 11.853 | -1.799 | 1.00 | 63.01 |
| ATOM | 1544 | CD1 | ILE | 1648 | 15.274 | 10.746 | -2.738 | 1.00 | 60.11 |
| ATOM | 1545 | C | ILE | 1648 | 15.542 | 13.990 | 0.046 | 1.00 | 71.12 |
| ATOM | 1546 | O | ILE | 1648 | 16.628 | 14.310 | 0.525 | 1.00 | 72.41 |
| ATOM | 1547 | N | HIS | 1649 | 14.923 | 14.710 | -0.883 | 1.00 | 73.09 |
| ATOM | 1549 | CA | HIS | 1649 | 15.546 | 15.890 | -1.469 | 1.00 | 74.66 |
| ATOM | 1550 | CB | HIS | 1649 | 14.921 | 16.191 | -2.835 | 1.00 | 76.00 |
| ATOM | 1551 | CG | HIS | 1649 | 15.178 | 15.157 | -3.867 | 1.00 | 78.03 |
| ATOM | 1552 | CD2 | HIS | 1649 | 16.314 | 14.425 | -4.151 | 1.00 | 78.85 |
| ATOM | 1553 | ND1 | HIS | 1649 | 14.245 | 14.739 | -4.795 | 1.00 | 78.49 |
| ATOM | 1555 | CE1 | HIS | 1649 | 14.765 | 13.835 | -5.584 | 1.00 | 78.94 |
| ATOM | 1556 | NE2 | HIS | 1649 | 16.005 | 13.623 | -5.226 | 1.00 | 78.22 |
| ATOM | 1558 | C | HIS | 1649 | 15.466 | 17.108 | -0.549 | 1.00 | 75.04 |
| ATOM | 1559 | O | HIS | 1649 | 15.567 | 18.244 | -1.007 | 1.00 | 75.49 |
| ATOM | 1560 | N | HIS | 1650 | 15.265 | 16.860 | 0.743 | 1.00 | 76.11 |
| ATOM | 1562 | CA | HIS | 1650 | 15.181 | 17.918 | 1.748 | 1.00 | 77.63 |
| ATOM | 1563 | CB | HIS | 1650 | 13.723 | 18.327 | 1.995 | 1.00 | 81.10 |
| ATOM | 1564 | CG | HIS | 1650 | 13.206 | 19.352 | 1.033 | 1.00 | 86.06 |
| ATOM | 1565 | CD2 | HIS | 1650 | 13.662 | 20.592 | 0.730 | 1.00 | 88.74 |
| ATOM | 1566 | ND1 | HIS | 1650 | 12.099 | 19.146 | 0.239 | 1.00 | 88.83 |
| ATOM | 1568 | CE1 | HIS | 1650 | 11.893 | 20.211 | -0.511 | 1.00 | 90.51 |
| ATOM | 1569 | NE2 | HIS | 1650 | 12.823 | 21.103 | -0.238 | 1.00 | 90.75 |
| ATOM | 1571 | C | HIS | 1650 | 15.824 | 17.482 | 3.064 | 1.00 | 77.39 |
| ATOM | 1572 | O | HIS | 1650 | 15.651 | 18.133 | 4.091 | 1.00 | 77.42 |
| ATOM | 1573 | N | ILE | 1651 | 16.573 | 16.385 | 3.024 | 1.00 | 77.73 |
| ATOM | 1575 | CA | ILE | 1651 | 17.241 | 15.864 | 4.212 | 1.00 | 77.02 |
| ATOM | 1576 | CB | ILE | 1651 | 17.788 | 14.433 | 3.974 | 1.00 | 78.24 |
| ATOM | 1577 | CG2 | ILE | 1651 | 18.647 | 13.963 | 5.153 | 1.00 | 77.92 |
| ATOM | 1578 | CG1 | ILE | 1651 | 16.633 | 13.458 | 3.750 | 1.00 | 80.90 |
| ATOM | 1579 | CD1 | ILE | 1651 | 17.094 | 12.032 | 3.483 | 1.00 | 82.41 |
| ATOM | 1580 | C | ILE | 1651 | 18.411 | 16.748 | 4.620 | 1.00 | 76.15 |
| ATOM | 1581 | O | ILE | 1651 | 19.269 | 17.078 | 3.803 | 1.00 | 76.52 |
| ATOM | 1582 | N | ASP | 1652 | 18.432 | 17.150 | 5.882 | 1.00 | 75.13 |
| ATOM | 1584 | CA | ASP | 1652 | 19.527 | 17.957 | 6.384 | 1.00 | 73.91 |
| ATOM | 1585 | CB | ASP | 1652 | 19.068 | 18.781 | 7.592 | 1.00 | 76.30 |
| ATOM | 1586 | CG | ASP | 1652 | 20.216 | 19.499 | 8.286 | 1.00 | 79.91 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1587 | OD1 | ASP | 1652 | 21.247 | 19.786 | 7.636 | 1.00 | 82.38 |
| ATOM | 1588 | OD2 | ASP | 1652 | 20.081 | 19.780 | 9.497 | 1.00 | 81.51 |
| ATOM | 1589 | C | ASP | 1652 | 20.637 | 16.984 | 6.783 | 1.00 | 72.31 |
| ATOM | 1590 | O | ASP | 1652 | 20.599 | 16.403 | 7.866 | 1.00 | 71.41 |
| ATOM | 1591 | N | TYR | 1653 | 21.610 | 16.805 | 5.894 | 1.00 | 71.44 |
| ATOM | 1593 | CA | TYR | 1653 | 22.736 | 15.900 | 6.143 | 1.00 | 70.07 |
| ATOM | 1594 | CB | TYR | 1653 | 23.655 | 15.849 | 4.921 | 1.00 | 66.96 |
| ATOM | 1595 | CG | TYR | 1653 | 23.153 | 14.932 | 3.834 | 1.00 | 66.43 |
| ATOM | 1596 | CD1 | TYR | 1653 | 23.881 | 14.757 | 2.657 | 1.00 | 66.60 |
| ATOM | 1597 | CE1 | TYR | 1653 | 23.434 | 13.898 | 1.653 | 1.00 | 68.33 |
| ATOM | 1598 | CD2 | TYR | 1653 | 21.960 | 14.224 | 3.981 | 1.00 | 66.58 |
| ATOM | 1599 | CE2 | TYR | 1653 | 21.500 | 13.363 | 2.990 | 1.00 | 68.84 |
| ATOM | 1600 | CZ | TYR | 1653 | 22.241 | 13.205 | 1.823 | 1.00 | 69.34 |
| ATOM | 1601 | OH | TYR | 1653 | 21.781 | 12.360 | 0.833 | 1.00 | 69.88 |
| ATOM | 1603 | C | TYR | 1653 | 23.557 | 16.227 | 7.391 | 1.00 | 70.80 |
| ATOM | 1604 | O | TYR | 1653 | 24.197 | 15.351 | 7.975 | 1.00 | 70.62 |
| ATOM | 1605 | N | TYR | 1654 | 23.531 | 17.488 | 7.802 | 1.00 | 70.76 |
| ATOM | 1607 | CA | TYR | 1654 | 24.280 | 17.902 | 8.972 | 1.00 | 70.97 |
| ATOM | 1608 | CB | TYR | 1654 | 24.795 | 19.328 | 8.783 | 1.00 | 69.27 |
| ATOM | 1609 | CG | TYR | 1654 | 25.935 | 19.401 | 7.787 | 1.00 | 69.68 |
| ATOM | 1610 | CD1 | TYR | 1654 | 25.696 | 19.352 | 6.415 | 1.00 | 69.51 |
| ATOM | 1611 | CE1 | TYR | 1654 | 26.750 | 19.380 | 5.498 | 1.00 | 70.15 |
| ATOM | 1612 | CD2 | TYR | 1654 | 27.256 | 19.482 | 8.221 | 1.00 | 69.92 |
| ATOM | 1613 | CE2 | TYR | 1654 | 28.314 | 19.513 | 7.316 | 1.00 | 70.26 |
| ATOM | 1614 | CZ | TYR | 1654 | 28.057 | 19.462 | 5.958 | 1.00 | 70.22 |
| ATOM | 1615 | OH | TYR | 1654 | 29.111 | 19.492 | 5.069 | 1.00 | 69.67 |
| ATOM | 1617 | C | TYR | 1654 | 23.503 | 17.763 | 10.272 | 1.00 | 72.19 |
| ATOM | 1618 | O | TYR | 1654 | 24.035 | 18.043 | 11.344 | 1.00 | 73.21 |
| ATOM | 1619 | N | LYS | 1655 | 22.269 | 17.275 | 10.183 | 1.00 | 73.05 |
| ATOM | 1621 | CA | LYS | 1655 | 21.424 | 17.108 | 11.363 | 1.00 | 74.81 |
| ATOM | 1622 | CB | LYS | 1655 | 19.955 | 17.124 | 10.953 | 1.00 | 75.63 |
| ATOM | 1623 | CG | LYS | 1655 | 18.978 | 17.239 | 12.102 | 1.00 | 79.16 |
| ATOM | 1624 | CD | LYS | 1655 | 17.581 | 17.513 | 11.576 | 1.00 | 84.09 |
| ATOM | 1625 | CE | LYS | 1655 | 16.517 | 17.244 | 12.634 | 1.00 | 87.56 |
| ATOM | 1626 | NZ | LYS | 1655 | 15.139 | 17.478 | 12.097 | 1.00 | 89.36 |
| ATOM | 1630 | C | LYS | 1655 | 21.738 | 15.834 | 12.156 | 1.00 | 75.72 |
| ATOM | 1631 | O | LYS | 1655 | 21.900 | 14.751 | 11.586 | 1.00 | 77.14 |
| ATOM | 1632 | N | LYS | 1656 | 21.815 | 15.977 | 13.477 | 1.00 | 75.08 |
| ATOM | 1634 | CA | LYS | 1656 | 22.106 | 14.857 | 14.363 | 1.00 | 73.36 |
| ATOM | 1635 | CB | LYS | 1656 | 23.062 | 15.296 | 15.477 | 1.00 | 72.88 |
| ATOM | 1636 | CG | LYS | 1656 | 24.475 | 15.599 | 15.007 | 1.00 | 72.87 |
| ATOM | 1637 | CD | LYS | 1656 | 25.346 | 16.048 | 16.167 | 1.00 | 74.66 |
| ATOM | 1638 | CE | LYS | 1656 | 26.830 | 15.945 | 15.828 | 1.00 | 74.84 |
| ATOM | 1639 | NZ | LYS | 1656 | 27.701 | 16.322 | 16.981 | 1.00 | 73.74 |
| ATOM | 1643 | C | LYS | 1656 | 20.827 | 14.311 | 14.982 | 1.00 | 72.45 |
| ATOM | 1644 | O | LYS | 1656 | 19.795 | 14.991 | 15.007 | 1.00 | 72.74 |
| ATOM | 1645 | N | THR | 1657 | 20.900 | 13.075 | 15.469 | 1.00 | 71.26 |
| ATOM | 1647 | CA | THR | 1657 | 19.763 | 12.426 | 16.107 | 1.00 | 70.05 |
| ATOM | 1648 | CB | THR | 1657 | 19.969 | 10.886 | 16.206 | 1.00 | 68.30 |
| ATOM | 1649 | OG1 | THR | 1657 | 21.084 | 10.598 | 17.060 | 1.00 | 69.34 |
| ATOM | 1651 | CG2 | THR | 1657 | 20.244 | 10.292 | 14.839 | 1.00 | 66.16 |
| ATOM | 1652 | C | THR | 1657 | 19.707 | 13.019 | 17.504 | 1.00 | 70.37 |
| ATOM | 1653 | O | THR | 1657 | 20.608 | 13.761 | 17.892 | 1.00 | 71.47 |
| ATOM | 1654 | N | THR | 1658 | 18.669 | 12.691 | 18.263 | 1.00 | 70.80 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1656 | CA | THR | 1658 | 18.559 | 13.205 | 19.626 | 1.00 | 71.54 |
| ATOM | 1657 | CB | THR | 1658 | 17.334 | 12.600 | 20.325 | 1.00 | 71.20 |
| ATOM | 1658 | C | THR | 1658 | 19.844 | 12.865 | 20.394 | 1.00 | 70.91 |
| ATOM | 1659 | O | THR | 1658 | 20.429 | 13.722 | 21.063 | 1.00 | 71.25 |
| ATOM | 1660 | N | ASN | 1659 | 20.331 | 11.639 | 20.199 | 1.00 | 68.87 |
| ATOM | 1662 | CA | ASN | 1659 | 21.537 | 11.157 | 20.871 | 1.00 | 65.52 |
| ATOM | 1663 | CB | ASN | 1659 | 21.602 | 9.635 | 20.796 | 1.00 | 67.39 |
| ATOM | 1664 | CG | ASN | 1659 | 22.419 | 9.032 | 21.916 | 1.00 | 69.42 |
| ATOM | 1665 | OD1 | ASN | 1659 | 22.261 | 9.410 | 23.076 | 1.00 | 71.70 |
| ATOM | 1666 | ND2 | ASN | 1659 | 23.278 | 8.069 | 21.583 | 1.00 | 68.93 |
| ATOM | 1669 | C | ASN | 1659 | 22.830 | 11.749 | 20.318 | 1.00 | 62.51 |
| ATOM | 1670 | O | ASN | 1659 | 23.917 | 11.351 | 20.733 | 1.00 | 61.47 |
| ATOM | 1671 | N | GLY | 1660 | 22.706 | 12.654 | 19.348 | 1.00 | 59.76 |
| ATOM | 1673 | CA | GLY | 1660 | 23.859 | 13.307 | 18.750 | 1.00 | 57.70 |
| ATOM | 1674 | C | GLY | 1660 | 24.553 | 12.593 | 17.597 | 1.00 | 56.98 |
| ATOM | 1675 | O | GLY | 1660 | 25.659 | 12.979 | 17.199 | 1.00 | 57.55 |
| ATOM | 1676 | N | ARG | 1661 | 23.909 | 11.573 | 17.037 | 1.00 | 55.34 |
| ATOM | 1678 | CA | ARG | 1661 | 24.504 | 10.826 | 15.928 | 1.00 | 52.28 |
| ATOM | 1679 | CB | ARG | 1661 | 24.255 | 9.334 | 16.092 | 1.00 | 50.68 |
| ATOM | 1680 | CG | ARG | 1661 | 24.811 | 8.744 | 17.365 | 1.00 | 49.61 |
| ATOM | 1681 | CD | ARG | 1661 | 24.542 | 7.267 | 17.361 | 1.00 | 52.30 |
| ATOM | 1682 | NE | ARG | 1661 | 24.942 | 6.599 | 18.595 | 1.00 | 53.64 |
| ATOM | 1684 | CZ | ARG | 1661 | 24.731 | 5.306 | 18.826 | 1.00 | 56.32 |
| ATOM | 1685 | NH1 | ARG | 1661 | 24.124 | 4.559 | 17.901 | 1.00 | 54.04 |
| ATOM | 1688 | NH2 | ARG | 1661 | 25.145 | 4.754 | 19.965 | 1.00 | 54.48 |
| ATOM | 1691 | C | ARG | 1661 | 24.015 | 11.288 | 14.560 | 1.00 | 49.89 |
| ATOM | 1692 | O | ARG | 1661 | 22.916 | 11.812 | 14.429 | 1.00 | 51.43 |
| ATOM | 1693 | N | LEU | 1662 | 24.839 | 11.080 | 13.542 | 1.00 | 45.78 |
| ATOM | 1695 | CA | LEU | 1662 | 24.503 | 11.481 | 12.186 | 1.00 | 43.05 |
| ATOM | 1696 | CB | LEU | 1662 | 25.762 | 12.020 | 11.492 | 1.00 | 42.15 |
| ATOM | 1697 | CG | LEU | 1662 | 26.351 | 13.306 | 12.088 | 1.00 | 40.60 |
| ATOM | 1698 | CD1 | LEU | 1662 | 27.780 | 13.512 | 11.641 | 1.00 | 38.14 |
| ATOM | 1699 | CD2 | LEU | 1662 | 25.484 | 14.499 | 11.705 | 1.00 | 42.00 |
| ATOM | 1700 | C | LEU | 1662 | 23.867 | 10.346 | 11.370 | 1.00 | 41.81 |
| ATOM | 1701 | O | LEU | 1662 | 24.548 | 9.406 | 10.957 | 1.00 | 40.46 |
| ATOM | 1702 | N | PRO | 1663 | 22.546 | 10.428 | 11.118 | 1.00 | 40.49 |
| ATOM | 1703 | CD | PRO | 1663 | 21.659 | 11.519 | 11.561 | 1.00 | 40.60 |
| ATOM | 1704 | CA | PRO | 1663 | 21.794 | 9.423 | 10.351 | 1.00 | 38.17 |
| ATOM | 1705 | CB | PRO | 1663 | 20.433 | 10.095 | 10.158 | 1.00 | 38.43 |
| ATOM | 1706 | CG | PRO | 1663 | 20.282 | 10.901 | 11.414 | 1.00 | 40.65 |
| ATOM | 1707 | C | PRO | 1663 | 22.445 | 9.059 | 9.012 | 1.00 | 35.40 |
| ATOM | 1708 | O | PRO | 1663 | 22.265 | 7.949 | 8.521 | 1.00 | 33.01 |
| ATOM | 1709 | N | VAL | 1664 | 23.200 | 9.989 | 8.426 | 1.00 | 34.56 |
| ATOM | 1711 | CA | VAL | 1664 | 23.889 | 9.722 | 7.160 | 1.00 | 32.91 |
| ATOM | 1712 | CB | VAL | 1664 | 24.757 | 10.916 | 6.659 | 1.00 | 33.13 |
| ATOM | 1713 | CG1 | VAL | 1664 | 23.912 | 11.929 | 5.968 | 1.00 | 33.44 |
| ATOM | 1714 | CG2 | VAL | 1664 | 25.521 | 11.554 | 7.792 | 1.00 | 33.68 |
| ATOM | 1715 | C | VAL | 1664 | 24.812 | 8.511 | 7.266 | 1.00 | 30.58 |
| ATOM | 1716 | O | VAL | 1664 | 25.157 | 7.903 | 6.257 | 1.00 | 29.20 |
| ATOM | 1717 | N | LYS | 1665 | 25.211 | 8.171 | 8.489 | 1.00 | 28.02 |
| ATOM | 1719 | CA | LYS | 1665 | 26.102 | 7.044 | 8.726 | 1.00 | 24.95 |
| ATOM | 1720 | CB | LYS | 1665 | 26.749 | 7.153 | 10.098 | 1.00 | 24.39 |
| ATOM | 1721 | CG | LYS | 1665 | 27.811 | 8.231 | 10.140 | 1.00 | 28.36 |
| ATOM | 1722 | CD | LYS | 1665 | 28.189 | 8.628 | 11.548 | 1.00 | 29.24 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1723 | CE | LYS | 1665 | 29.269 | 9.690 | 11.489 | 1.00 | 31.15 |
| ATOM | 1724 | NZ | LYS | 1665 | 29.639 | 10.194 | 12.836 | 1.00 | 35.47 |
| ATOM | 1728 | C | LYS | 1665 | 25.440 | 5.692 | 8.543 | 1.00 | 25.16 |
| ATOM | 1729 | O | LYS | 1665 | 26.096 | 4.671 | 8.627 | 1.00 | 24.34 |
| ATOM | 1730 | N | TRP | 1666 | 24.138 | 5.698 | 8.286 | 1.00 | 25.16 |
| ATOM | 1732 | CA | TRP | 1666 | 23.414 | 4.461 | 8.053 | 1.00 | 26.61 |
| ATOM | 1733 | CB | TRP | 1666 | 22.157 | 4.412 | 8.917 | 1.00 | 28.17 |
| ATOM | 1734 | CG | TRP | 1666 | 22.428 | 3.931 | 10.330 | 1.00 | 30.26 |
| ATOM | 1735 | CD2 | TRP | 1666 | 22.930 | 4.714 | 11.426 | 1.00 | 26.92 |
| ATOM | 1736 | CE2 | TRP | 1666 | 23.063 | 3.837 | 12.537 | 1.00 | 26.34 |
| ATOM | 1737 | CE3 | TRP | 1666 | 23.286 | 6.057 | 11.598 | 1.00 | 24.69 |
| ATOM | 1738 | CD1 | TRP | 1666 | 22.276 | 2.656 | 10.800 | 1.00 | 26.44 |
| ATOM | 1739 | NE1 | TRP | 1666 | 22.659 | 2.592 | 12.118 | 1.00 | 25.65 |
| ATOM | 1741 | CZ2 | TRP | 1666 | 23.535 | 4.264 | 13.779 | 1.00 | 24.97 |
| ATOM | 1742 | CZ3 | TRP | 1666 | 23.758 | 6.484 | 12.837 | 1.00 | 22.23 |
| ATOM | 1743 | CH2 | TRP | 1666 | 23.877 | 5.587 | 13.908 | 1.00 | 24.97 |
| ATOM | 1744 | C | TRP | 1666 | 23.048 | 4.345 | 6.572 | 1.00 | 27.24 |
| ATOM | 1745 | O | TRP | 1666 | 22.573 | 3.301 | 6.116 | 1.00 | 29.16 |
| ATOM | 1746 | N | MET | 1667 | 23.355 | 5.390 | 5.811 | 1.00 | 26.70 |
| ATOM | 1748 | CA | MET | 1667 | 23.022 | 5.444 | 4.398 | 1.00 | 25.21 |
| ATOM | 1749 | CB | MET | 1667 | 22.828 | 6.893 | 3.963 | 1.00 | 28.81 |
| ATOM | 1750 | CG | MET | 1667 | 21.704 | 7.630 | 4.637 | 1.00 | 35.42 |
| ATOM | 1751 | SD | MET | 1667 | 21.567 | 9.283 | 3.924 | 1.00 | 42.64 |
| ATOM | 1752 | CE | MET | 1667 | 20.959 | 8.858 | 2.369 | 1.00 | 41.32 |
| ATOM | 1753 | C | MET | 1667 | 23.984 | 4.807 | 3.417 | 1.00 | 25.03 |
| ATOM | 1754 | O | MET | 1667 | 25.182 | 5.047 | 3.446 | 1.00 | 24.24 |
| ATOM | 1755 | N | ALA | 1668 | 23.420 | 4.034 | 2.501 | 1.00 | 26.70 |
| ATOM | 1757 | CA | ALA | 1668 | 24.186 | 3.398 | 1.441 | 1.00 | 27.82 |
| ATOM | 1758 | CB | ALA | 1668 | 23.272 | 2.509 | 0.601 | 1.00 | 25.36 |
| ATOM | 1759 | C | ALA | 1668 | 24.738 | 4.528 | 0.575 | 1.00 | 28.42 |
| ATOM | 1760 | O | ALA | 1668 | 24.044 | 5.521 | 0.321 | 1.00 | 27.52 |
| ATOM | 1761 | N | PRO | 1669 | 25.972 | 4.374 | 0.065 | 1.00 | 28.95 |
| ATOM | 1762 | CD | PRO | 1669 | 26.867 | 3.214 | 0.170 | 1.00 | 27.98 |
| ATOM | 1763 | CA | PRO | 1669 | 26.571 | 5.418 | -0.775 | 1.00 | 28.76 |
| ATOM | 1764 | CB | PRO | 1669 | 27.814 | 4.731 | -1.326 | 1.00 | 28.58 |
| ATOM | 1765 | CG | PRO | 1669 | 28.193 | 3.809 | -0.209 | 1.00 | 30.22 |
| ATOM | 1766 | C | PRO | 1669 | 25.647 | 5.909 | -1.893 | 1.00 | 27.08 |
| ATOM | 1767 | O | PRO | 1669 | 25.496 | 7.107 | -2.093 | 1.00 | 28.31 |
| ATOM | 1768 | N | GLU | 1670 | 24.993 | 4.997 | -2.595 | 1.00 | 25.42 |
| ATOM | 1770 | CA | GLU | 1670 | 24.110 | 5.423 | -3.673 | 1.00 | 27.02 |
| ATOM | 1771 | CB | GLU | 1670 | 23.680 | 4.233 | -4.542 | 1.00 | 27.18 |
| ATOM | 1772 | CG | GLU | 1670 | 22.662 | 3.294 | -3.911 | 1.00 | 27.66 |
| ATOM | 1773 | CD | GLU | 1670 | 23.280 | 2.162 | -3.112 | 1.00 | 27.75 |
| ATOM | 1774 | OE1 | GLU | 1670 | 22.488 | 1.309 | -2.647 | 1.00 | 27.12 |
| ATOM | 1775 | OE2 | GLU | 1670 | 24.526 | 2.114 | -2.944 | 1.00 | 21.64 |
| ATOM | 1776 | C | GLU | 1670 | 22.896 | 6.229 | -3.189 | 1.00 | 26.88 |
| ATOM | 1777 | O | GLU | 1670 | 22.348 | 7.037 | -3.929 | 1.00 | 24.52 |
| ATOM | 1778 | N | ALA | 1671 | 22.477 | 6.009 | -1.948 | 1.00 | 29.43 |
| ATOM | 1780 | CA | ALA | 1671 | 21.342 | 6.744 | -1.392 | 1.00 | 29.29 |
| ATOM | 1781 | CB | ALA | 1671 | 20.751 | 5.989 | -0.217 | 1.00 | 26.98 |
| ATOM | 1782 | C | ALA | 1671 | 21.826 | 8.124 | -0.939 | 1.00 | 31.14 |
| ATOM | 1783 | O | ALA | 1671 | 21.159 | 9.135 | -1.143 | 1.00 | 31.67 |
| ATOM | 1784 | N | LEU | 1672 | 23.013 | 8.139 | -0.343 | 1.00 | 32.31 |
| ATOM | 1786 | CA | LEU | 1672 | 23.636 | 9.352 | 0.154 | 1.00 | 33.79 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1787 | CB | LEU | 1672 | 24.841 | 8.986 | 1.008 | 1.00 | 34.49 |
| ATOM | 1788 | CG | LEU | 1672 | 25.585 | 10.166 | 1.618 | 1.00 | 37.16 |
| ATOM | 1789 | CD1 | LEU | 1672 | 24.713 | 10.840 | 2.666 | 1.00 | 42.22 |
| ATOM | 1790 | CD2 | LEU | 1672 | 26.863 | 9.665 | 2.237 | 1.00 | 33.93 |
| ATOM | 1791 | C | LEU | 1672 | 24.078 | 10.280 | -0.972 | 1.00 | 36.30 |
| ATOM | 1792 | O | LEU | 1672 | 23.789 | 11.478 | -0.949 | 1.00 | 39.09 |
| ATOM | 1793 | N | PHE | 1673 | 24.770 | 9.723 | -1.957 | 1.00 | 34.39 |
| ATOM | 1795 | CA | PHE | 1673 | 25.266 | 10.504 | -3.075 | 1.00 | 33.81 |
| ATOM | 1796 | CB | PHE | 1673 | 26.553 | 9.874 | -3.625 | 1.00 | 33.15 |
| ATOM | 1797 | CG | PHE | 1673 | 27.661 | 9.761 | -2.617 | 1.00 | 33.44 |
| ATOM | 1798 | CD1 | PHE | 1673 | 28.313 | 8.545 | -2.419 | 1.00 | 32.17 |
| ATOM | 1799 | CD2 | PHE | 1673 | 28.055 | 10.867 | -1.861 | 1.00 | 34.87 |
| ATOM | 1800 | CE1 | PHE | 1673 | 29.346 | 8.419 | -1.484 | 1.00 | 31.98 |
| ATOM | 1801 | CE2 | PHE | 1673 | 29.090 | 10.757 | -0.919 | 1.00 | 36.31 |
| ATOM | 1802 | CZ | PHE | 1673 | 29.736 | 9.525 | -0.732 | 1.00 | 34.55 |
| ATOM | 1803 | C | PHE | 1673 | 24.273 | 10.670 | -4.217 | 1.00 | 34.79 |
| ATOM | 1804 | O | PHE | 1673 | 24.135 | 11.754 | -4.765 | 1.00 | 35.74 |
| ATOM | 1805 | N | ASP | 1674 | 23.584 | 9.588 | -4.572 | 1.00 | 37.31 |
| ATOM | 1807 | CA | ASP | 1674 | 22.650 | 9.601 | -5.698 | 1.00 | 35.61 |
| ATOM | 1808 | CB | ASP | 1674 | 22.917 | 8.392 | -6.600 | 1.00 | 37.01 |
| ATOM | 1809 | CG | ASP | 1674 | 24.362 | 8.288 | -7.041 | 1.00 | 41.02 |
| ATOM | 1810 | OD1 | ASP | 1674 | 25.030 | 9.340 | -7.194 | 1.00 | 43.07 |
| ATOM | 1811 | OD2 | ASP | 1674 | 24.828 | 7.145 | -7.251 | 1.00 | 42.24 |
| ATOM | 1812 | C | ASP | 1674 | 21.162 | 9.632 | -5.360 | 1.00 | 37.06 |
| ATOM | 1813 | O | ASP | 1674 | 20.315 | 9.506 | -6.257 | 1.00 | 36.37 |
| ATOM | 1814 | N | ARG | 1675 | 20.840 | 9.745 | -4.077 | 1.00 | 37.78 |
| ATOM | 1816 | CA | ARG | 1675 | 19.445 | 9.791 | -3.650 | 1.00 | 39.41 |
| ATOM | 1817 | CB | ARG | 1675 | 18.832 | 11.137 | -4.039 | 1.00 | 44.39 |
| ATOM | 1818 | CG | ARG | 1675 | 19.413 | 12.299 | -3.269 | 1.00 | 54.30 |
| ATOM | 1819 | CD | ARG | 1675 | 19.516 | 13.551 | -4.127 | 1.00 | 63.84 |
| ATOM | 1820 | NE | ARG | 1675 | 20.060 | 14.664 | -3.349 | 1.00 | 73.69 |
| ATOM | 1822 | CZ | ARG | 1675 | 19.652 | 15.925 | -3.453 | 1.00 | 77.10 |
| ATOM | 1823 | NH1 | ARG | 1675 | 18.695 | 16.253 | -4.312 | 1.00 | 79.65 |
| ATOM | 1826 | NH2 | ARG | 1675 | 20.177 | 16.855 | -2.665 | 1.00 | 79.31 |
| ATOM | 1829 | C | ARG | 1675 | 18.617 | 8.639 | -4.221 | 1.00 | 37.46 |
| ATOM | 1830 | O | ARG | 1675 | 17.447 | 8.808 | -4.557 | 1.00 | 38.57 |
| ATOM | 1831 | N | ILE | 1676 | 19.235 | 7.475 | -4.351 | 1.00 | 34.37 |
| ATOM | 1833 | CA | ILE | 1676 | 18.545 | 6.313 | -4.874 | 1.00 | 32.99 |
| ATOM | 1834 | CB | ILE | 1676 | 19.358 | 5.644 | -5.976 | 1.00 | 33.98 |
| ATOM | 1835 | CG2 | ILE | 1676 | 18.552 | 4.529 | -6.602 | 1.00 | 35.04 |
| ATOM | 1836 | CG1 | ILE | 1676 | 19.708 | 6.663 | -7.050 | 1.00 | 34.92 |
| ATOM | 1837 | CD1 | ILE | 1676 | 20.799 | 6.200 | -7.962 | 1.00 | 41.16 |
| ATOM | 1838 | C | ILE | 1676 | 18.315 | 5.315 | -3.743 | 1.00 | 31.55 |
| ATOM | 1839 | O | ILE | 1676 | 19.245 | 4.632 | -3.300 | 1.00 | 30.65 |
| ATOM | 1840 | N | TYR | 1677 | 17.082 | 5.279 | -3.246 | 1.00 | 30.88 |
| ATOM | 1842 | CA | TYR | 1677 | 16.701 | 4.371 | -2.173 | 1.00 | 27.10 |
| ATOM | 1843 | CB | TYR | 1677 | 15.771 | 5.074 | -1.208 | 1.00 | 28.30 |
| ATOM | 1844 | CG | TYR | 1677 | 16.457 | 6.136 | -0.406 | 1.00 | 30.61 |
| ATOM | 1845 | CD1 | TYR | 1677 | 16.598 | 7.432 | -0.905 | 1.00 | 30.82 |
| ATOM | 1846 | CE1 | TYR | 1677 | 17.212 | 8.424 | -0.159 | 1.00 | 30.75 |
| ATOM | 1847 | CD2 | TYR | 1677 | 16.952 | 5.857 | 0.863 | 1.00 | 29.75 |
| ATOM | 1848 | CE2 | TYR | 1677 | 17.567 | 6.842 | 1.621 | 1.00 | 32.62 |
| ATOM | 1849 | CZ | TYR | 1677 | 17.688 | 8.125 | 1.110 | 1.00 | 34.51 |
| ATOM | 1850 | OH | TYR | 1677 | 18.238 | 9.118 | 1.888 | 1.00 | 38.89 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1852 | C | TYR | 1677 | 16.029 | 3.149 | -2.743 | 1.00 | 25.47 |
| ATOM | 1853 | O | TYR | 1677 | 15.132 | 3.264 | -3.578 | 1.00 | 26.00 |
| ATOM | 1854 | N | THR | 1678 | 16.459 | 1.983 | -2.272 | 1.00 | 24.27 |
| ATOM | 1856 | CA | THR | 1678 | 15.942 | 0.701 | -2.734 | 1.00 | 24.09 |
| ATOM | 1857 | CB | THR | 1678 | 16.830 | 0.123 | -3.853 | 1.00 | 24.19 |
| ATOM | 1858 | OG1 | THR | 1678 | 18.165 | -0.008 | -3.349 | 1.00 | 27.81 |
| ATOM | 1860 | CG2 | THR | 1678 | 16.843 | 1.009 | -5.085 | 1.00 | 24.15 |
| ATOM | 1861 | C | THR | 1678 | 15.979 | -0.297 | -1.577 | 1.00 | 25.02 |
| ATOM | 1862 | O | THR | 1678 | 16.379 | 0.036 | -0.465 | 1.00 | 27.65 |
| ATOM | 1863 | N | HIS | 1679 | 15.569 | -1.530 | -1.844 | 1.00 | 25.04 |
| ATOM | 1865 | CA | HIS | 1679 | 15.591 | -2.560 | -0.818 | 1.00 | 24.35 |
| ATOM | 1866 | CB | HIS | 1679 | 14.853 | -3.812 | -1.298 | 1.00 | 23.78 |
| ATOM | 1867 | CG | HIS | 1679 | 13.390 | -3.592 | -1.536 | 1.00 | 27.24 |
| ATOM | 1868 | CD2 | HIS | 1679 | 12.627 | -3.758 | -2.643 | 1.00 | 28.22 |
| ATOM | 1869 | ND1 | HIS | 1679 | 12.532 | -3.137 | -0.551 | 1.00 | 30.64 |
| ATOM | 1871 | CE1 | HIS | 1679 | 11.310 | -3.028 | -1.041 | 1.00 | 28.13 |
| ATOM | 1872 | NE2 | HIS | 1679 | 11.339 | -3.400 | -2.307 | 1.00 | 28.52 |
| ATOM | 1874 | C | HIS | 1679 | 17.056 | -2.846 | -0.514 | 1.00 | 22.52 |
| ATOM | 1875 | O | HIS | 1679 | 17.419 | -3.179 | 0.613 | 1.00 | 22.58 |
| ATOM | 1876 | N | GLN | 1680 | 17.898 | -2.604 | -1.516 | 1.00 | 24.34 |
| ATOM | 1878 | CA | GLN | 1680 | 19.341 | -2.800 | -1.406 | 1.00 | 23.52 |
| ATOM | 1879 | CB | GLN | 1680 | 19.998 | -2.781 | -2.782 | 1.00 | 25.36 |
| ATOM | 1880 | CG | GLN | 1680 | 19.741 | -4.050 | -3.577 | 1.00 | 33.28 |
| ATOM | 1881 | CD | GLN | 1680 | 19.212 | -3.763 | -4.949 | 1.00 | 34.68 |
| ATOM | 1882 | OE1 | GLN | 1680 | 18.683 | -2.686 | -5.187 | 1.00 | 41.24 |
| ATOM | 1883 | NE2 | GLN | 1680 | 19.357 | -4.713 | -5.867 | 1.00 | 32.10 |
| ATOM | 1886 | C | GLN | 1680 | 19.998 | -1.767 | -0.514 | 1.00 | 23.38 |
| ATOM | 1887 | O | GLN | 1680 | 20.925 | -2.094 | 0.224 | 1.00 | 25.12 |
| ATOM | 1888 | N | SER | 1681 | 19.533 | -0.521 | -0.562 | 1.00 | 20.87 |
| ATOM | 1890 | CA | SER | 1681 | 20.133 | 0.480 | 0.303 | 1.00 | 20.53 |
| ATOM | 1891 | CB | SER | 1681 | 19.821 | 1.919 | -0.151 | 1.00 | 19.58 |
| ATOM | 1892 | OG | SER | 1681 | 18.445 | 2.126 | -0.425 | 1.00 | 20.67 |
| ATOM | 1894 | C | SER | 1681 | 19.696 | 0.189 | 1.741 | 1.00 | 22.22 |
| ATOM | 1895 | O | SER | 1681 | 20.439 | 0.455 | 2.681 | 1.00 | 23.62 |
| ATOM | 1896 | N | ASP | 1682 | 18.530 | -0.436 | 1.900 | 1.00 | 22.44 |
| ATOM | 1898 | CA | ASP | 1682 | 18.054 | -0.816 | 3.231 | 1.00 | 22.70 |
| ATOM | 1899 | CB | ASP | 1682 | 16.607 | -1.293 | 3.180 | 1.00 | 24.24 |
| ATOM | 1900 | CG | ASP | 1682 | 15.603 | -0.165 | 3.352 | 1.00 | 28.23 |
| ATOM | 1901 | OD1 | ASP | 1682 | 14.410 | -0.425 | 3.108 | 1.00 | 28.14 |
| ATOM | 1902 | OD2 | ASP | 1682 | 15.976 | 0.960 | 3.757 | 1.00 | 25.23 |
| ATOM | 1903 | C | ASP | 1682 | 18.926 | -1.941 | 3.777 | 1.00 | 23.92 |
| ATOM | 1904 | O | ASP | 1682 | 19.121 | -2.057 | 4.990 | 1.00 | 26.24 |
| ATOM | 1905 | N | VAL | 1683 | 19.433 | -2.788 | 2.884 | 1.00 | 23.67 |
| ATOM | 1907 | CA | VAL | 1683 | 20.300 | -3.888 | 3.302 | 1.00 | 22.42 |
| ATOM | 1908 | CB | VAL | 1683 | 20.562 | -4.881 | 2.141 | 1.00 | 23.70 |
| ATOM | 1909 | CG1 | VAL | 1683 | 21.724 | -5.802 | 2.459 | 1.00 | 19.73 |
| ATOM | 1910 | CG2 | VAL | 1683 | 19.292 | -5.713 | 1.889 | 1.00 | 19.85 |
| ATOM | 1911 | C | VAL | 1683 | 21.584 | -3.298 | 3.860 | 1.00 | 21.94 |
| ATOM | 1912 | O | VAL | 1683 | 22.030 | -3.688 | 4.938 | 1.00 | 22.69 |
| ATOM | 1913 | N | TRP | 1684 | 22.141 | -2.320 | 3.154 | 1.00 | 20.51 |
| ATOM | 1915 | CA | TRP | 1684 | 23.349 | -1.633 | 3.611 | 1.00 | 20.31 |
| ATOM | 1916 | CB | TRP | 1684 | 23.659 | -0.446 | 2.680 | 1.00 | 19.01 |
| ATOM | 1917 | CG | TRP | 1684 | 24.802 | 0.410 | 3.145 | 1.00 | 20.67 |
| ATOM | 1918 | CD2 | TRP | 1684 | 26.114 | 0.468 | 2.587 | 1.00 | 22.26 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1919 | CE2 | TRP | 1684 | 26.890 | 1.316 | 3.408 | 1.00 | 21.22 |
| ATOM | 1920 | CE3 | TRP | 1684 | 26.718 | -0.127 | 1.463 | 1.00 | 22.51 |
| ATOM | 1921 | CD1 | TRP | 1684 | 24.825 | 1.229 | 4.248 | 1.00 | 19.91 |
| ATOM | 1922 | NE1 | TRP | 1684 | 26.079 | 1.763 | 4.414 | 1.00 | 18.59 |
| ATOM | 1924 | CZ2 | TRP | 1684 | 28.236 | 1.586 | 3.148 | 1.00 | 20.81 |
| ATOM | 1925 | CZ3 | TRP | 1684 | 28.059 | 0.141 | 1.204 | 1.00 | 22.01 |
| ATOM | 1926 | CH2 | TRP | 1684 | 28.806 | 0.992 | 2.047 | 1.00 | 23.34 |
| ATOM | 1927 | C | TRP | 1684 | 23.131 | -1.150 | 5.069 | 1.00 | 21.49 |
| ATOM | 1928 | O | TRP | 1684 | 23.958 | -1.412 | 5.954 | 1.00 | 23.34 |
| ATOM | 1929 | N | SER | 1685 | 22.015 | -0.463 | 5.308 | 1.00 | 21.84 |
| ATOM | 1931 | CA | SER | 1685 | 21.652 | 0.042 | 6.634 | 1.00 | 20.02 |
| ATOM | 1932 | CB | SER | 1685 | 20.310 | 0.773 | 6.559 | 1.00 | 19.12 |
| ATOM | 1933 | OG | SER | 1685 | 20.335 | 1.791 | 5.578 | 1.00 | 21.62 |
| ATOM | 1935 | C | SER | 1685 | 21.551 | -1.111 | 7.648 | 1.00 | 22.64 |
| ATOM | 1936 | O | SER | 1685 | 21.908 | -0.946 | 8.829 | 1.00 | 22.09 |
| ATOM | 1937 | N | PHE | 1686 | 21.043 | -2.266 | 7.202 | 1.00 | 22.44 |
| ATOM | 1939 | CA | PHE | 1686 | 20.939 | -3.438 | 8.075 | 1.00 | 22.91 |
| ATOM | 1940 | CB | PHE | 1686 | 20.196 | -4.588 | 7.380 | 1.00 | 23.75 |
| ATOM | 1941 | CG | PHE | 1686 | 20.027 | -5.808 | 8.256 | 1.00 | 23.61 |
| ATOM | 1942 | CD1 | PHE | 1686 | 19.220 | -5.757 | 9.388 | 1.00 | 21.21 |
| ATOM | 1943 | CD2 | PHE | 1686 | 20.731 | -6.976 | 7.990 | 1.00 | 23.91 |
| ATOM | 1944 | CE1 | PHE | 1686 | 19.118 | -6.836 | 10.240 | 1.00 | 20.66 |
| ATOM | 1945 | CE2 | PHE | 1686 | 20.636 | -8.074 | 8.841 | 1.00 | 22.47 |
| ATOM | 1946 | CZ | PHE | 1686 | 19.828 | -7.999 | 9.972 | 1.00 | 23.35 |
| ATOM | 1947 | C | PHE | 1686 | 22.339 | -3.904 | 8.522 | 1.00 | 22.60 |
| ATOM | 1948 | O | PHE | 1686 | 22.526 | -4.382 | 9.646 | 1.00 | 22.83 |
| ATOM | 1949 | N | GLY | 1687 | 23.312 | -3.770 | 7.626 | 1.00 | 23.82 |
| ATOM | 1951 | CA | GLY | 1687 | 24.682 | -4.140 | 7.941 | 1.00 | 22.58 |
| ATOM | 1952 | C | GLY | 1687 | 25.175 | -3.262 | 9.071 | 1.00 | 21.49 |
| ATOM | 1953 | O | GLY | 1687 | 25.832 | -3.749 | 9.990 | 1.00 | 21.62 |
| ATOM | 1954 | N | VAL | 1688 | 24.849 | -1.968 | 9.008 | 1.00 | 21.15 |
| ATOM | 1956 | CA | VAL | 1688 | 25.229 | -1.008 | 10.052 | 1.00 | 20.56 |
| ATOM | 1957 | CB | VAL | 1688 | 24.894 | 0.479 | 9.647 | 1.00 | 17.69 |
| ATOM | 1958 | CG1 | VAL | 1688 | 25.408 | 1.456 | 10.690 | 1.00 | 15.11 |
| ATOM | 1959 | CG2 | VAL | 1688 | 25.518 | 0.821 | 8.314 | 1.00 | 11.54 |
| ATOM | 1960 | C | VAL | 1688 | 24.494 | -1.398 | 11.346 | 1.00 | 22.60 |
| ATOM | 1961 | O | VAL | 1688 | 25.083 | -1.407 | 12.428 | 1.00 | 25.23 |
| ATOM | 1962 | N | LEU | 1689 | 23.215 | -1.755 | 11.229 | 1.00 | 26.09 |
| ATOM | 1964 | CA | LEU | 1689 | 22.423 | -2.175 | 12.387 | 1.00 | 25.16 |
| ATOM | 1965 | CB | LEU | 1689 | 20.976 | -2.455 | 11.965 | 1.00 | 25.91 |
| ATOM | 1966 | CG | LEU | 1689 | 19.913 | -2.560 | 13.068 | 1.00 | 27.54 |
| ATOM | 1967 | CD1 | LEU | 1689 | 18.557 | -2.241 | 12.496 | 1.00 | 28.11 |
| ATOM | 1968 | CD2 | LEU | 1689 | 19.898 | -3.940 | 13.704 | 1.00 | 31.67 |
| ATOM | 1969 | C | LEU | 1689 | 23.055 | -3.426 | 13.018 | 1.00 | 27.49 |
| ATOM | 1970 | O | LEU | 1689 | 23.128 | -3.532 | 14.246 | 1.00 | 28.99 |
| ATOM | 1971 | N | LEU | 1690 | 23.485 | -4.374 | 12.180 | 1.00 | 27.67 |
| ATOM | 1973 | CA | LEU | 1690 | 24.149 | -5.596 | 12.643 | 1.00 | 26.76 |
| ATOM | 1974 | CB | LEU | 1690 | 24.616 | -6.453 | 11.456 | 1.00 | 28.58 |
| ATOM | 1975 | CG | LEU | 1690 | 23.651 | -7.406 | 10.733 | 1.00 | 29.46 |
| ATOM | 1976 | CD1 | LEU | 1690 | 24.372 | -8.064 | 9.565 | 1.00 | 27.79 |
| ATOM | 1977 | CD2 | LEU | 1690 | 23.130 | -8.488 | 11.691 | 1.00 | 28.15 |
| ATOM | 1978 | C | LEU | 1690 | 25.362 | -5.176 | 13.476 | 1.00 | 26.19 |
| ATOM | 1979 | O | LEU | 1690 | 25.565 | -5.670 | 14.597 | 1.00 | 25.29 |
| ATOM | 1980 | N | TRP | 1691 | 26.124 | -4.217 | 12.946 | 1.00 | 25.89 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1982 | CA | TRP | 1691 | 27.302 | -3.682 | 13.631 | 1.00 | 27.31 |
| ATOM | 1983 | CB | TRP | 1691 | 27.979 | -2.628 | 12.755 | 1.00 | 25.21 |
| ATOM | 1984 | CG | TRP | 1691 | 29.338 | -2.170 | 13.257 | 1.00 | 27.00 |
| ATOM | 1985 | CD2 | TRP | 1691 | 29.606 | -1.060 | 14.134 | 1.00 | 24.28 |
| ATOM | 1986 | CE2 | TRP | 1691 | 31.001 | -0.988 | 14.297 | 1.00 | 23.03 |
| ATOM | 1987 | CE3 | TRP | 1691 | 28.792 | -0.118 | 14.778 | 1.00 | 22.80 |
| ATOM | 1988 | CD1 | TRP | 1691 | 30.562 | -2.712 | 12.944 | 1.00 | 24.10 |
| ATOM | 1989 | NE1 | TRP | 1691 | 31.557 | -2.010 | 13.567 | 1.00 | 23.41 |
| ATOM | 1991 | CZ2 | TRP | 1691 | 31.617 | -0.011 | 15.097 | 1.00 | 25.00 |
| ATOM | 1992 | CZ3 | TRP | 1691 | 29.398 | 0.851 | 15.573 | 1.00 | 26.78 |
| ATOM | 1993 | CH2 | TRP | 1691 | 30.802 | 0.900 | 15.719 | 1.00 | 27.78 |
| ATOM | 1994 | C | TRP | 1691 | 26.947 | -3.088 | 15.012 | 1.00 | 28.70 |
| ATOM | 1995 | O | TRP | 1691 | 27.708 | -3.245 | 15.974 | 1.00 | 29.56 |
| ATOM | 1996 | N | GLU | 1692 | 25.808 | -2.400 | 15.104 | 1.00 | 29.51 |
| ATOM | 1998 | CA | GLU | 1692 | 25.349 | -1.817 | 16.371 | 1.00 | 27.55 |
| ATOM | 1999 | CB | GLU | 1692 | 24.120 | -0.935 | 16.171 | 1.00 | 28.35 |
| ATOM | 2000 | CG | GLU | 1692 | 24.273 | 0.221 | 15.219 | 1.00 | 24.70 |
| ATOM | 2001 | CD | GLU | 1692 | 22.982 | 0.989 | 15.100 | 1.00 | 25.44 |
| ATOM | 2002 | OE1 | GLU | 1692 | 22.224 | 0.744 | 14.148 | 1.00 | 24.34 |
| ATOM | 2003 | OE2 | GLU | 1692 | 22.696 | 1.816 | 15.982 | 1.00 | 27.57 |
| ATOM | 2004 | C | GLU | 1692 | 24.958 | -2.918 | 17.352 | 1.00 | 28.74 |
| ATOM | 2005 | O | GLU | 1692 | 25.099 | -2.753 | 18.557 | 1.00 | 28.76 |
| ATOM | 2006 | N | ILE | 1693 | 24.421 | -4.023 | 16.844 | 1.00 | 29.23 |
| ATOM | 2008 | CA | ILE | 1693 | 24.027 | -5.125 | 17.712 | 1.00 | 27.48 |
| ATOM | 2009 | CB | ILE | 1693 | 23.205 | -6.226 | 16.944 | 1.00 | 26.80 |
| ATOM | 2010 | CG2 | ILE | 1693 | 22.983 | -7.469 | 17.842 | 1.00 | 22.98 |
| ATOM | 2011 | CG1 | ILE | 1693 | 21.840 | -5.658 | 16.508 | 1.00 | 27.36 |
| ATOM | 2012 | CD1 | ILE | 1693 | 21.005 | -6.585 | 15.635 | 1.00 | 24.84 |
| ATOM | 2013 | C | ILE | 1693 | 25.259 | -5.750 | 18.357 | 1.00 | 27.27 |
| ATOM | 2014 | O | ILE | 1693 | 25.320 | -5.902 | 19.575 | 1.00 | 28.15 |
| ATOM | 2015 | N | PHE | 1694 | 26.273 | -6.043 | 17.552 | 1.00 | 27.83 |
| ATOM | 2017 | CA | PHE | 1694 | 27.473 | -6.677 | 18.095 | 1.00 | 29.88 |
| ATOM | 2018 | CB | PHE | 1694 | 28.143 | -7.525 | 17.011 | 1.00 | 28.66 |
| ATOM | 2019 | CG | PHE | 1694 | 27.223 | -8.574 | 16.463 | 1.00 | 29.92 |
| ATOM | 2020 | CD1 | PHE | 1694 | 26.628 | -8.424 | 15.220 | 1.00 | 30.20 |
| ATOM | 2021 | CD2 | PHE | 1694 | 26.809 | -9.630 | 17.269 | 1.00 | 30.81 |
| ATOM | 2022 | CE1 | PHE | 1694 | 25.625 | -9.294 | 14.801 | 1.00 | 32.42 |
| ATOM | 2023 | CE2 | PHE | 1694 | 25.805 | -10.508 | 16.857 | 1.00 | 32.30 |
| ATOM | 2024 | CZ | PHE | 1694 | 25.210 | -10.337 | 15.628 | 1.00 | 31.13 |
| ATOM | 2025 | C | PHE | 1694 | 28.429 | -5.784 | 18.890 | 1.00 | 31.07 |
| ATOM | 2026 | O | PHE | 1694 | 29.376 | -6.273 | 19.509 | 1.00 | 33.16 |
| ATOM | 2027 | N | THR | 1695 | 28.157 | -4.480 | 18.897 | 1.00 | 29.20 |
| ATOM | 2029 | CA | THR | 1695 | 28.934 | -3.532 | 19.670 | 1.00 | 27.38 |
| ATOM | 2030 | CB | THR | 1695 | 29.412 | -2.333 | 18.823 | 1.00 | 24.77 |
| ATOM | 2031 | OG1 | THR | 1695 | 28.287 | -1.652 | 18.274 | 1.00 | 26.27 |
| ATOM | 2033 | CG2 | THR | 1695 | 30.305 | -2.800 | 17.706 | 1.00 | 20.18 |
| ATOM | 2034 | C | THR | 1695 | 28.053 | -3.034 | 20.822 | 1.00 | 29.84 |
| ATOM | 2035 | O | THR | 1695 | 28.430 | -2.103 | 21.548 | 1.00 | 32.77 |
| ATOM | 2036 | N | LEU | 1696 | 26.898 | -3.687 | 20.988 | 1.00 | 28.52 |
| ATOM | 2038 | CA | LEU | 1696 | 25.915 | -3.364 | 22.029 | 1.00 | 28.82 |
| ATOM | 2039 | CB | LEU | 1696 | 26.356 | -3.886 | 23.394 | 1.00 | 32.50 |
| ATOM | 2040 | CG | LEU | 1696 | 26.658 | -5.379 | 23.476 | 1.00 | 33.24 |
| ATOM | 2041 | CD1 | LEU | 1696 | 27.205 | -5.717 | 24.849 | 1.00 | 34.15 |
| ATOM | 2042 | CD2 | LEU | 1696 | 25.398 | -6.150 | 23.191 | 1.00 | 37.24 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2043 | C | LEU | 1696 | 25.553 | -1.888 | 22.131 | 1.00 | 26.98 |
| ATOM | 2044 | O | LEU | 1696 | 25.579 | -1.297 | 23.207 | 1.00 | 27.59 |
| ATOM | 2045 | N | GLY | 1697 | 25.148 | -1.317 | 21.007 | 1.00 | 27.86 |
| ATOM | 2047 | CA | GLY | 1697 | 24.767 | 0.074 | 20.980 | 1.00 | 27.40 |
| ATOM | 2048 | C | GLY | 1697 | 25.927 | 0.962 | 20.618 | 1.00 | 27.47 |
| ATOM | 2049 | O | GLY | 1697 | 25.957 | 2.132 | 20.998 | 1.00 | 28.78 |
| ATOM | 2050 | N | GLY | 1698 | 26.888 | 0.416 | 19.885 | 1.00 | 27.26 |
| ATOM | 2052 | CA | GLY | 1698 | 28.031 | 1.212 | 19.482 | 1.00 | 29.54 |
| ATOM | 2053 | C | GLY | 1698 | 27.651 | 2.301 | 18.492 | 1.00 | 31.17 |
| ATOM | 2054 | O | GLY | 1698 | 26.669 | 2.177 | 17.755 | 1.00 | 33.73 |
| ATOM | 2055 | N | SER | 1699 | 28.418 | 3.380 | 18.481 | 1.00 | 29.96 |
| ATOM | 2057 | CA | SER | 1699 | 28.168 | 4.491 | 17.577 | 1.00 | 29.37 |
| ATOM | 2058 | CB | SER | 1699 | 28.438 | 5.810 | 18.319 | 1.00 | 31.77 |
| ATOM | 2059 | OG | SER | 1699 | 28.575 | 6.919 | 17.431 | 1.00 | 38.42 |
| ATOM | 2061 | C | SER | 1699 | 29.093 | 4.350 | 16.369 | 1.00 | 27.98 |
| ATOM | 2062 | O | SER | 1699 | 30.299 | 4.310 | 16.529 | 1.00 | 28.18 |
| ATOM | 2063 | N | PRO | 1700 | 28.537 | 4.240 | 15.153 | 1.00 | 29.62 |
| ATOM | 2064 | CD | PRO | 1700 | 27.104 | 4.259 | 14.794 | 1.00 | 31.22 |
| ATOM | 2065 | CA | PRO | 1700 | 29.381 | 4.107 | 13.958 | 1.00 | 28.95 |
| ATOM | 2066 | CB | PRO | 1700 | 28.356 | 4.003 | 12.807 | 1.00 | 27.21 |
| ATOM | 2067 | CG | PRO | 1700 | 27.095 | 3.556 | 13.460 | 1.00 | 29.33 |
| ATOM | 2068 | C | PRO | 1700 | 30.205 | 5.379 | 13.773 | 1.00 | 28.78 |
| ATOM | 2069 | O | PRO | 1700 | 29.737 | 6.469 | 14.110 | 1.00 | 30.04 |
| ATOM | 2070 | N | TYR | 1701 | 31.426 | 5.239 | 13.264 | 1.00 | 28.35 |
| ATOM | 2072 | CA | TYR | 1701 | 32.296 | 6.390 | 12.987 | 1.00 | 30.77 |
| ATOM | 2073 | CB | TYR | 1701 | 31.921 | 6.987 | 11.615 | 1.00 | 31.67 |
| ATOM | 2074 | CG | TYR | 1701 | 32.060 | 6.037 | 10.454 | 1.00 | 34.61 |
| ATOM | 2075 | CD1 | TYR | 1701 | 30.952 | 5.673 | 9.686 | 1.00 | 38.26 |
| ATOM | 2076 | CE1 | TYR | 1701 | 31.083 | 4.806 | 8.587 | 1.00 | 40.99 |
| ATOM | 2077 | CD2 | TYR | 1701 | 33.301 | 5.520 | 10.106 | 1.00 | 38.16 |
| ATOM | 2078 | CE2 | TYR | 1701 | 33.449 | 4.662 | 9.020 | 1.00 | 41.04 |
| ATOM | 2079 | CZ | TYR | 1701 | 32.343 | 4.312 | 8.263 | 1.00 | 43.11 |
| ATOM | 2080 | OH | TYR | 1701 | 32.531 | 3.478 | 7.181 | 1.00 | 49.53 |
| ATOM | 2082 | C | TYR | 1701 | 32.305 | 7.532 | 14.029 | 1.00 | 31.41 |
| ATOM | 2083 | O | TYR | 1701 | 32.026 | 8.689 | 13.698 | 1.00 | 33.59 |
| ATOM | 2084 | N | PRO | 1702 | 32.635 | 7.230 | 15.296 | 1.00 | 30.92 |
| ATOM | 2085 | CD | PRO | 1702 | 32.998 | 5.938 | 15.888 | 1.00 | 32.30 |
| ATOM | 2086 | CA | PRO | 1702 | 32.656 | 8.283 | 16.314 | 1.00 | 30.05 |
| ATOM | 2087 | CB | PRO | 1702 | 33.123 | 7.548 | 17.561 | 1.00 | 27.77 |
| ATOM | 2088 | CG | PRO | 1702 | 32.676 | 6.174 | 17.338 | 1.00 | 32.34 |
| ATOM | 2089 | C | PRO | 1702 | 33.659 | 9.366 | 15.944 | 1.00 | 31.42 |
| ATOM | 2090 | O | PRO | 1702 | 34.769 | 9.055 | 15.513 | 1.00 | 30.95 |
| ATOM | 2091 | N | GLY | 1703 | 33.257 | 10.627 | 16.117 | 1.00 | 31.30 |
| ATOM | 2093 | CA | GLY | 1703 | 34.122 | 11.751 | 15.817 | 1.00 | 29.66 |
| ATOM | 2094 | C | GLY | 1703 | 34.172 | 12.138 | 14.351 | 1.00 | 31.00 |
| ATOM | 2095 | O | GLY | 1703 | 34.752 | 13.165 | 13.999 | 1.00 | 30.69 |
| ATOM | 2096 | N | VAL | 1704 | 33.551 | 11.331 | 13.491 | 1.00 | 31.11 |
| ATOM | 2098 | CA | VAL | 1704 | 33.553 | 11.610 | 12.059 | 1.00 | 29.88 |
| ATOM | 2099 | CB | VAL | 1704 | 33.539 | 10.310 | 11.244 | 1.00 | 28.41 |
| ATOM | 2100 | CG1 | VAL | 1704 | 33.585 | 10.624 | 9.750 | 1.00 | 26.24 |
| ATOM | 2101 | CG2 | VAL | 1704 | 34.702 | 9.429 | 11.649 | 1.00 | 24.10 |
| ATOM | 2102 | C | VAL | 1704 | 32.396 | 12.508 | 11.604 | 1.00 | 30.80 |
| ATOM | 2103 | O | VAL | 1704 | 31.224 | 12.146 | 11.712 | 1.00 | 32.50 |
| ATOM | 2104 | N | PRO | 1705 | 32.718 | 13.705 | 11.104 | 1.00 | 30.86 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2105 | CD | PRO | 1705 | 34.039 | 14.350 | 11.077 | 1.00 | 30.59 |
| ATOM | 2106 | CA | PRO | 1705 | 31.682 | 14.625 | 10.645 | 1.00 | 31.47 |
| ATOM | 2107 | CB | PRO | 1705 | 32.400 | 15.971 | 10.680 | 1.00 | 32.75 |
| ATOM | 2108 | CG | PRO | 1705 | 33.774 | 15.607 | 10.289 | 1.00 | 32.59 |
| ATOM | 2109 | C | PRO | 1705 | 31.258 | 14.264 | 9.239 | 1.00 | 32.19 |
| ATOM | 2110 | O | PRO | 1705 | 31.974 | 13.536 | 8.549 | 1.00 | 33.91 |
| ATOM | 2111 | N | VAL | 1706 | 30.124 | 14.814 | 8.806 | 1.00 | 32.57 |
| ATOM | 2113 | CA | VAL | 1706 | 29.560 | 14.576 | 7.474 | 1.00 | 31.80 |
| ATOM | 2114 | CB | VAL | 1706 | 28.483 | 15.632 | 7.172 | 1.00 | 34.66 |
| ATOM | 2115 | CG1 | VAL | 1706 | 28.022 | 15.538 | 5.738 | 1.00 | 39.06 |
| ATOM | 2116 | CG2 | VAL | 1706 | 27.309 | 15.455 | 8.106 | 1.00 | 36.62 |
| ATOM | 2117 | C | VAL | 1706 | 30.578 | 14.560 | 6.320 | 1.00 | 31.58 |
| ATOM | 2118 | O | VAL | 1706 | 30.682 | 13.585 | 5.570 | 1.00 | 32.35 |
| ATOM | 2119 | N | GLU | 1707 | 31.326 | 15.649 | 6.189 | 1.00 | 31.46 |
| ATOM | 2121 | CA | GLU | 1707 | 32.329 | 15.788 | 5.139 | 1.00 | 31.68 |
| ATOM | 2122 | CB | GLU | 1707 | 33.021 | 17.148 | 5.267 | 1.00 | 32.59 |
| ATOM | 2123 | C | GLU | 1707 | 33.381 | 14.678 | 5.114 | 1.00 | 32.23 |
| ATOM | 2124 | O | GLU | 1707 | 33.740 | 14.183 | 4.050 | 1.00 | 33.47 |
| ATOM | 2125 | N | GLU | 1708 | 33.902 | 14.316 | 6.279 | 1.00 | 32.90 |
| ATOM | 2127 | CA | GLU | 1708 | 34.909 | 13.268 | 6.352 | 1.00 | 33.86 |
| ATOM | 2128 | CB | GLU | 1708 | 35.570 | 13.244 | 7.730 | 1.00 | 38.54 |
| ATOM | 2129 | CG | GLU | 1708 | 36.190 | 14.575 | 8.165 | 1.00 | 47.63 |
| ATOM | 2130 | CD | GLU | 1708 | 37.442 | 14.962 | 7.383 | 1.00 | 58.35 |
| ATOM | 2131 | OE1 | GLU | 1708 | 38.117 | 14.067 | 6.816 | 1.00 | 62.88 |
| ATOM | 2132 | OE2 | GLU | 1708 | 37.770 | 16.176 | 7.355 | 1.00 | 64.79 |
| ATOM | 2133 | C | GLU | 1708 | 34.276 | 11.921 | 6.043 | 1.00 | 33.56 |
| ATOM | 2134 | O | GLU | 1708 | 34.927 | 11.038 | 5.489 | 1.00 | 34.18 |
| ATOM | 2135 | N | LEU | 1709 | 32.997 | 11.774 | 6.374 | 1.00 | 32.91 |
| ATOM | 2137 | CA | LEU | 1709 | 32.285 | 10.532 | 6.108 | 1.00 | 33.83 |
| ATOM | 2138 | CB | LEU | 1709 | 30.862 | 10.563 | 6.685 | 1.00 | 32.28 |
| ATOM | 2139 | CG | LEU | 1709 | 30.015 | 9.363 | 6.231 | 1.00 | 32.92 |
| ATOM | 2140 | CD1 | LEU | 1709 | 30.541 | 8.071 | 6.853 | 1.00 | 28.37 |
| ATOM | 2141 | CD2 | LEU | 1709 | 28.563 | 9.580 | 6.568 | 1.00 | 31.90 |
| ATOM | 2142 | C | LEU | 1709 | 32.222 | 10.283 | 4.606 | 1.00 | 34.15 |
| ATOM | 2143 | O | LEU | 1709 | 32.412 | 9.152 | 4.156 | 1.00 | 34.75 |
| ATOM | 2144 | N | PHE | 1710 | 31.918 | 11.332 | 3.844 | 1.00 | 33.83 |
| ATOM | 2146 | CA | PHE | 1710 | 31.828 | 11.248 | 2.388 | 1.00 | 32.90 |
| ATOM | 2147 | CB | PHE | 1710 | 31.531 | 12.622 | 1.787 | 1.00 | 34.85 |
| ATOM | 2148 | CG | PHE | 1710 | 30.162 | 13.132 | 2.082 | 1.00 | 38.60 |
| ATOM | 2149 | CD1 | PHE | 1710 | 29.150 | 12.268 | 2.469 | 1.00 | 43.69 |
| ATOM | 2150 | CD2 | PHE | 1710 | 29.882 | 14.480 | 1.984 | 1.00 | 45.10 |
| ATOM | 2151 | CE1 | PHE | 1710 | 27.873 | 12.742 | 2.764 | 1.00 | 46.23 |
| ATOM | 2152 | CE2 | PHE | 1710 | 28.611 | 14.966 | 2.274 | 1.00 | 48.15 |
| ATOM | 2153 | CZ | PHE | 1710 | 27.603 | 14.086 | 2.670 | 1.00 | 46.90 |
| ATOM | 2154 | C | PHE | 1710 | 33.131 | 10.739 | 1.803 | 1.00 | 31.84 |
| ATOM | 2155 | O | PHE | 1710 | 33.134 | 9.931 | 0.877 | 1.00 | 29.97 |
| ATOM | 2156 | N | LYS | 1711 | 34.231 | 11.224 | 2.373 | 1.00 | 32.45 |
| ATOM | 2158 | CA | LYS | 1711 | 35.582 | 10.860 | 1.947 | 1.00 | 34.53 |
| ATOM | 2159 | CB | LYS | 1711 | 36.588 | 11.755 | 2.675 | 1.00 | 36.17 |
| ATOM | 2160 | CG | LYS | 1711 | 38.008 | 11.669 | 2.182 | 1.00 | 41.07 |
| ATOM | 2161 | CD | LYS | 1711 | 38.912 | 12.582 | 3.001 | 1.00 | 46.23 |
| ATOM | 2162 | CE | LYS | 1711 | 40.311 | 12.648 | 2.418 | 1.00 | 51.79 |
| ATOM | 2163 | NZ | LYS | 1711 | 41.036 | 11.360 | 2.556 | 1.00 | 57.27 |
| ATOM | 2167 | C | LYS | 1711 | 35.867 | 9.375 | 2.215 | 1.00 | 33.82 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2168 | O | LYS | 1711 | 36.451 | 8.688 | 1.376 | 1.00 | 33.20 |
| ATOM | 2169 | N | LEU | 1712 | 35.439 | 8.885 | 3.382 | 1.00 | 34.52 |
| ATOM | 2171 | CA | LEU | 1712 | 35.618 | 7.477 | 3.754 | 1.00 | 33.25 |
| ATOM | 2172 | CB | LEU | 1712 | 35.094 | 7.211 | 5.189 | 1.00 | 30.99 |
| ATOM | 2173 | CG | LEU | 1712 | 35.746 | 7.917 | 6.393 | 1.00 | 29.71 |
| ATOM | 2174 | CD1 | LEU | 1712 | 35.047 | 7.552 | 7.678 | 1.00 | 24.11 |
| ATOM | 2175 | CD2 | LEU | 1712 | 37.208 | 7.552 | 6.497 | 1.00 | 32.21 |
| ATOM | 2176 | C | LEU | 1712 | 34.833 | 6.631 | 2.744 | 1.00 | 32.16 |
| ATOM | 2177 | O | LEU | 1712 | 35.378 | 5.732 | 2.109 | 1.00 | 32.77 |
| ATOM | 2178 | N | LEU | 1713 | 33.562 | 6.967 | 2.563 | 1.00 | 31.72 |
| ATOM | 2180 | CA | LEU | 1713 | 32.700 | 6.259 | 1.637 | 1.00 | 33.60 |
| ATOM | 2181 | CB | LEU | 1713 | 31.299 | 6.879 | 1.619 | 1.00 | 36.57 |
| ATOM | 2182 | CG | LEU | 1713 | 30.522 | 6.711 | 2.930 | 1.00 | 37.60 |
| ATOM | 2183 | CD1 | LEU | 1713 | 29.284 | 7.575 | 2.927 | 1.00 | 35.03 |
| ATOM | 2184 | CD2 | LEU | 1713 | 30.182 | 5.246 | 3.157 | 1.00 | 33.22 |
| ATOM | 2185 | C | LEU | 1713 | 33.285 | 6.248 | 0.236 | 1.00 | 35.33 |
| ATOM | 2186 | O | LEU | 1713 | 33.318 | 5.203 | -0.407 | 1.00 | 36.00 |
| ATOM | 2187 | N | LYS | 1714 | 33.741 | 7.405 | -0.234 | 1.00 | 36.24 |
| ATOM | 2189 | CA | LYS | 1714 | 34.331 | 7.501 | -1.566 | 1.00 | 36.35 |
| ATOM | 2190 | CB | LYS | 1714 | 34.707 | 8.946 | -1.900 | 1.00 | 35.82 |
| ATOM | 2191 | CG | LYS | 1714 | 33.520 | 9.837 | -2.168 | 1.00 | 37.23 |
| ATOM | 2192 | CD | LYS | 1714 | 32.712 | 9.324 | -3.337 | 1.00 | 40.53 |
| ATOM | 2193 | CE | LYS | 1714 | 31.506 | 10.198 | -3.600 | 1.00 | 44.51 |
| ATOM | 2194 | NZ | LYS | 1714 | 30.747 | 9.724 | -4.804 | 1.00 | 50.76 |
| ATOM | 2198 | C | LYS | 1714 | 35.559 | 6.613 | -1.701 | 1.00 | 37.60 |
| ATOM | 2199 | O | LYS | 1714 | 35.808 | 6.039 | -2.764 | 1.00 | 40.82 |
| ATOM | 2200 | N | GLU | 1715 | 36.299 | 6.452 | -0.615 | 1.00 | 35.61 |
| ATOM | 2202 | CA | GLU | 1715 | 37.496 | 5.630 | -0.658 | 1.00 | 34.65 |
| ATOM | 2203 | CB | GLU | 1715 | 38.517 | 6.188 | 0.320 | 1.00 | 37.83 |
| ATOM | 2204 | CG | GLU | 1715 | 38.897 | 7.613 | -0.036 | 1.00 | 42.28 |
| ATOM | 2205 | CD | GLU | 1715 | 39.634 | 8.342 | 1.061 | 1.00 | 45.64 |
| ATOM | 2206 | OE1 | GLU | 1715 | 39.928 | 7.726 | 2.114 | 1.00 | 43.09 |
| ATOM | 2207 | OE2 | GLU | 1715 | 39.918 | 9.544 | 0.853 | 1.00 | 47.56 |
| ATOM | 2208 | C | GLU | 1715 | 37.244 | 4.145 | -0.419 | 1.00 | 32.94 |
| ATOM | 2209 | O | GLU | 1715 | 38.177 | 3.348 | -0.419 | 1.00 | 33.31 |
| ATOM | 2210 | N | GLY | 1716 | 35.983 | 3.779 | -0.213 | 1.00 | 29.12 |
| ATOM | 2212 | CA | GLY | 1716 | 35.634 | 2.391 | 0.004 | 1.00 | 26.02 |
| ATOM | 2213 | C | GLY | 1716 | 35.946 | 1.895 | 1.396 | 1.00 | 29.60 |
| ATOM | 2214 | O | GLY | 1716 | 36.223 | 0.715 | 1.588 | 1.00 | 29.81 |
| ATOM | 2215 | N | HIS | 1717 | 35.879 | 2.783 | 2.379 | 1.00 | 29.97 |
| ATOM | 2217 | CA | HIS | 1717 | 36.158 | 2.409 | 3.763 | 1.00 | 30.78 |
| ATOM | 2218 | CB | HIS | 1717 | 36.369 | 3.659 | 4.623 | 1.00 | 33.25 |
| ATOM | 2219 | CG | HIS | 1717 | 36.653 | 3.360 | 6.067 | 1.00 | 34.70 |
| ATOM | 2220 | CD2 | HIS | 1717 | 37.820 | 3.155 | 6.715 | 1.00 | 32.77 |
| ATOM | 2221 | ND1 | HIS | 1717 | 35.656 | 3.219 | 7.010 | 1.00 | 36.90 |
| ATOM | 2223 | CE1 | HIS | 1717 | 36.200 | 2.932 | 8.180 | 1.00 | 35.87 |
| ATOM | 2224 | NE2 | HIS | 1717 | 37.513 | 2.887 | 8.027 | 1.00 | 31.93 |
| ATOM | 2226 | C | HIS | 1717 | 35.035 | 1.577 | 4.375 | 1.00 | 29.63 |
| ATOM | 2227 | O | HIS | 1717 | 33.861 | 1.847 | 4.133 | 1.00 | 30.82 |
| ATOM | 2228 | N | ARG | 1718 | 35.406 | 0.600 | 5.201 | 1.00 | 27.92 |
| ATOM | 2230 | CA | ARG | 1718 | 34.436 | -0.258 | 5.878 | 1.00 | 27.30 |
| ATOM | 2231 | CB | ARG | 1718 | 34.379 | -1.641 | 5.236 | 1.00 | 24.10 |
| ATOM | 2232 | CG | ARG | 1718 | 33.939 | -1.655 | 3.789 | 1.00 | 26.52 |
| ATOM | 2233 | CD | ARG | 1718 | 32.469 | -1.288 | 3.627 | 1.00 | 26.96 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2234 | NE | ARG | 1718 | 32.020 | -1.374 | 2.232 | 1.00 | 24.41 |
| ATOM | 2236 | CZ | ARG | 1718 | 32.090 | -0.377 | 1.352 | 1.00 | 25.51 |
| ATOM | 2237 | NH1 | ARG | 1718 | 32.611 | 0.801 | 1.706 | 1.00 | 23.61 |
| ATOM | 2240 | NH2 | ARG | 1718 | 31.553 | -0.521 | 0.149 | 1.00 | 21.28 |
| ATOM | 2243 | C | ARG | 1718 | 34.881 | -0.384 | 7.330 | 1.00 | 28.81 |
| ATOM | 2244 | O | ARG | 1718 | 36.080 | -0.425 | 7.611 | 1.00 | 29.77 |
| ATOM | 2245 | N | MET | 1719 | 33.920 | -0.377 | 8.250 | 1.00 | 30.40 |
| ATOM | 2247 | CA | MET | 1719 | 34.215 | -0.485 | 9.673 | 1.00 | 30.62 |
| ATOM | 2248 | CB | MET | 1719 | 32.942 | -0.339 | 10.497 | 1.00 | 28.91 |
| ATOM | 2249 | CG | MET | 1719 | 32.235 | 1.003 | 10.316 | 1.00 | 30.85 |
| ATOM | 2250 | SD | MET | 1719 | 30.829 | 1.237 | 11.432 | 1.00 | 33.27 |
| ATOM | 2251 | CE | MET | 1719 | 29.521 | 0.416 | 10.561 | 1.00 | 31.81 |
| ATOM | 2252 | C | MET | 1719 | 34.900 | -1.793 | 10.005 | 1.00 | 31.32 |
| ATOM | 2253 | O | MET | 1719 | 34.755 | -2.769 | 9.278 | 1.00 | 31.47 |
| ATOM | 2254 | N | ASP | 1720 | 35.651 | -1.799 | 11.103 | 1.00 | 33.78 |
| ATOM | 2256 | CA | ASP | 1720 | 36.387 | -2.983 | 11.550 | 1.00 | 33.45 |
| ATOM | 2257 | CB | ASP | 1720 | 37.478 | -2.580 | 12.546 | 1.00 | 36.99 |
| ATOM | 2258 | CG | ASP | 1720 | 38.585 | -1.762 | 11.908 | 1.00 | 41.56 |
| ATOM | 2259 | OD1 | ASP | 1720 | 38.403 | -1.339 | 10.742 | 1.00 | 48.43 |
| ATOM | 2260 | OD2 | ASP | 1720 | 39.634 | -1.546 | 12.568 | 1.00 | 40.99 |
| ATOM | 2261 | C | ASP | 1720 | 35.473 | -4.001 | 12.211 | 1.00 | 32.12 |
| ATOM | 2262 | O | ASP | 1720 | 34.381 | -3.657 | 12.668 | 1.00 | 30.89 |
| ATOM | 2263 | N | LYS | 1721 | 35.944 | -5.241 | 12.328 | 1.00 | 31.82 |
| ATOM | 2265 | CA | LYS | 1721 | 35.127 | -6.270 | 12.953 | 1.00 | 31.71 |
| ATOM | 2266 | CB | LYS | 1721 | 35.691 | -7.679 | 12.747 | 1.00 | 32.34 |
| ATOM | 2267 | CG | LYS | 1721 | 34.762 | -8.738 | 13.344 | 1.00 | 34.85 |
| ATOM | 2268 | CD | LYS | 1721 | 35.111 | -10.155 | 12.961 | 1.00 | 37.39 |
| ATOM | 2269 | CE | LYS | 1721 | 36.266 | -10.674 | 13.765 | 1.00 | 41.42 |
| ATOM | 2270 | NZ | LYS | 1721 | 36.348 | -12.154 | 13.635 | 1.00 | 46.55 |
| ATOM | 2274 | C | LYS | 1721 | 35.007 | -6.018 | 14.430 | 1.00 | 33.40 |
| ATOM | 2275 | O | LYS | 1721 | 36.017 | -5.879 | 15.121 | 1.00 | 34.26 |
| ATOM | 2276 | N | PRO | 1722 | 33.768 | -5.924 | 14.934 | 1.00 | 34.26 |
| ATOM | 2277 | CD | PRO | 1722 | 32.494 | -6.002 | 14.203 | 1.00 | 32.16 |
| ATOM | 2278 | CA | PRO | 1722 | 33.546 | -5.692 | 16.362 | 1.00 | 35.84 |
| ATOM | 2279 | CB | PRO | 1722 | 32.027 | -5.682 | 16.473 | 1.00 | 35.35 |
| ATOM | 2280 | CG | PRO | 1722 | 31.575 | -5.255 | 15.108 | 1.00 | 35.35 |
| ATOM | 2281 | C | PRO | 1722 | 34.105 | -6.904 | 17.099 | 1.00 | 40.41 |
| ATOM | 2282 | O | PRO | 1722 | 34.010 | -8.038 | 16.607 | 1.00 | 41.14 |
| ATOM | 2283 | N | SER | 1723 | 34.739 | -6.680 | 18.240 | 1.00 | 43.60 |
| ATOM | 2285 | CA | SER | 1723 | 35.260 | -7.808 | 18.999 | 1.00 | 45.51 |
| ATOM | 2286 | CB | SER | 1723 | 36.078 | -7.324 | 20.191 | 1.00 | 45.30 |
| ATOM | 2287 | OG | SER | 1723 | 35.384 | -6.300 | 20.879 | 1.00 | 49.62 |
| ATOM | 2289 | C | SER | 1723 | 34.031 | -8.589 | 19.460 | 1.00 | 46.39 |
| ATOM | 2290 | O | SER | 1723 | 32.939 | -8.028 | 19.614 | 1.00 | 45.16 |
| ATOM | 2291 | N | ASN | 1724 | 34.199 | -9.891 | 19.631 | 1.00 | 48.53 |
| ATOM | 2293 | CA | ASN | 1724 | 33.088 | -10.723 | 20.065 | 1.00 | 51.13 |
| ATOM | 2294 | CB | ASN | 1724 | 32.509 | -10.194 | 21.390 | 1.00 | 56.87 |
| ATOM | 2295 | CG | ASN | 1724 | 33.595 | -9.892 | 22.427 | 1.00 | 61.65 |
| ATOM | 2296 | OD1 | ASN | 1724 | 34.503 | -10.702 | 22.649 | 1.00 | 63.73 |
| ATOM | 2297 | ND2 | ASN | 1724 | 33.526 | -8.713 | 23.039 | 1.00 | 64.64 |
| ATOM | 2300 | C | ASN | 1724 | 32.034 | -10.743 | 18.941 | 1.00 | 48.83 |
| ATOM | 2301 | O | ASN | 1724 | 30.846 | -10.534 | 19.145 | 1.00 | 50.50 |
| ATOM | 2302 | N | CYS | 1725 | 32.511 | -10.977 | 17.734 | 1.00 | 45.23 |
| ATOM | 2304 | CA | CYS | 1725 | 31.654 | -11.056 | 16.570 | 1.00 | 42.33 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2305 | CB | CYS | 1725 | 31.570 | -9.702 | 15.854 | 1.00 | 41.48 |
| ATOM | 2306 | SG | CYS | 1725 | 30.711 | -9.751 | 14.275 | 1.00 | 40.38 |
| ATOM | 2307 | C | CYS | 1725 | 32.383 | -12.077 | 15.725 | 1.00 | 39.64 |
| ATOM | 2308 | O | CYS | 1725 | 33.601 | -12.004 | 15.579 | 1.00 | 42.00 |
| ATOM | 2309 | N | THR | 1726 | 31.664 | -13.090 | 15.263 | 1.00 | 35.96 |
| ATOM | 2311 | CA | THR | 1726 | 32.275 | -14.139 | 14.459 | 1.00 | 33.61 |
| ATOM | 2312 | CB | THR | 1726 | 31.301 | -15.326 | 14.326 | 1.00 | 33.29 |
| ATOM | 2313 | OG1 | THR | 1726 | 30.071 | -14.904 | 13.711 | 1.00 | 34.53 |
| ATOM | 2315 | CG2 | THR | 1726 | 30.981 | -15.861 | 15.696 | 1.00 | 25.84 |
| ATOM | 2316 | C | THR | 1726 | 32.720 | -13.629 | 13.092 | 1.00 | 32.27 |
| ATOM | 2317 | O | THR | 1726 | 32.257 | -12.593 | 12.643 | 1.00 | 33.04 |
| ATOM | 2318 | N | ASN | 1727 | 33.643 | -14.315 | 12.434 | 1.00 | 32.98 |
| ATOM | 2320 | CA | ASN | 1727 | 34.050 | -13.850 | 11.114 | 1.00 | 34.97 |
| ATOM | 2321 | CB | ASN | 1727 | 35.198 | -14.680 | 10.541 | 1.00 | 39.89 |
| ATOM | 2322 | CG | ASN | 1727 | 36.540 | -14.271 | 11.103 | 1.00 | 45.37 |
| ATOM | 2323 | OD1 | ASN | 1727 | 37.044 | -13.177 | 10.826 | 1.00 | 48.43 |
| ATOM | 2324 | ND2 | ASN | 1727 | 37.125 | -15.141 | 11.909 | 1.00 | 45.88 |
| ATOM | 2327 | C | ASN | 1727 | 32.846 | -13.947 | 10.192 | 1.00 | 33.97 |
| ATOM | 2328 | O | ASN | 1727 | 32.646 | -13.088 | 9.341 | 1.00 | 35.07 |
| ATOM | 2329 | N | GLU | 1728 | 32.024 | -14.973 | 10.414 | 1.00 | 31.69 |
| ATOM | 2331 | CA | GLU | 1728 | 30.814 | -15.210 | 9.620 | 1.00 | 30.27 |
| ATOM | 2332 | CB | GLU | 1728 | 30.141 | -16.493 | 10.083 | 1.00 | 32.53 |
| ATOM | 2333 | CG | GLU | 1728 | 28.932 | -16.878 | 9.273 | 1.00 | 32.81 |
| ATOM | 2334 | CD | GLU | 1728 | 28.353 | -18.190 | 9.711 | 1.00 | 36.43 |
| ATOM | 2335 | OE1 | GLU | 1728 | 28.339 | -18.466 | 10.932 | 1.00 | 36.75 |
| ATOM | 2336 | OE2 | GLU | 1728 | 27.908 | -18.945 | 8.829 | 1.00 | 41.92 |
| ATOM | 2337 | C | GLU | 1728 | 29.814 | -14.049 | 9.681 | 1.00 | 28.70 |
| ATOM | 2338 | O | GLU | 1728 | 29.234 | -13.655 | 8.660 | 1.00 | 28.51 |
| ATOM | 2339 | N | LEU | 1729 | 29.594 | -13.517 | 10.880 | 1.00 | 26.77 |
| ATOM | 2341 | CA | LEU | 1729 | 28.687 | -12.393 | 11.040 | 1.00 | 26.80 |
| ATOM | 2342 | CB | LEU | 1729 | 28.228 | -12.274 | 12.490 | 1.00 | 27.91 |
| ATOM | 2343 | CG | LEU | 1729 | 27.233 | -13.355 | 12.913 | 1.00 | 30.71 |
| ATOM | 2344 | CD1 | LEU | 1729 | 27.095 | -13.345 | 14.428 | 1.00 | 35.79 |
| ATOM | 2345 | CD2 | LEU | 1729 | 25.885 | -13.141 | 12.253 | 1.00 | 25.70 |
| ATOM | 2346 | C | LEU | 1729 | 29.319 | -11.089 | 10.540 | 1.00 | 27.06 |
| ATOM | 2347 | O | LEU | 1729 | 28.610 | -10.177 | 10.126 | 1.00 | 30.27 |
| ATOM | 2348 | N | TYR | 1730 | 30.650 | -11.004 | 10.549 | 1.00 | 27.03 |
| ATOM | 2350 | CA | TYR | 1730 | 31.328 | -9.812 | 10.039 | 1.00 | 26.21 |
| ATOM | 2351 | CB | TYR | 1730 | 32.792 | -9.778 | 10.474 | 1.00 | 25.31 |
| ATOM | 2352 | CG | TYR | 1730 | 33.538 | -8.553 | 9.982 | 1.00 | 24.89 |
| ATOM | 2353 | CD1 | TYR | 1730 | 33.012 | -7.270 | 10.169 | 1.00 | 23.59 |
| ATOM | 2354 | CE1 | TYR | 1730 | 33.655 | -6.148 | 9.665 | 1.00 | 24.74 |
| ATOM | 2355 | CD2 | TYR | 1730 | 34.739 | -8.675 | 9.285 | 1.00 | 22.11 |
| ATOM | 2356 | CE2 | TYR | 1730 | 35.399 | -7.560 | 8.775 | 1.00 | 22.32 |
| ATOM | 2357 | CZ | TYR | 1730 | 34.853 | -6.295 | 8.962 | 1.00 | 26.07 |
| ATOM | 2358 | OH | TYR | 1730 | 35.484 | -5.181 | 8.418 | 1.00 | 22.70 |
| ATOM | 2360 | C | TYR | 1730 | 31.227 | -9.878 | 8.509 | 1.00 | 27.71 |
| ATOM | 2361 | O | TYR | 1730 | 30.960 | -8.875 | 7.843 | 1.00 | 28.05 |
| ATOM | 2362 | N | MET | 1731 | 31.409 | -11.081 | 7.977 | 1.00 | 27.92 |
| ATOM | 2364 | CA | MET | 1731 | 31.306 | -11.355 | 6.548 | 1.00 | 28.89 |
| ATOM | 2365 | CB | MET | 1731 | 31.506 | -12.853 | 6.317 | 1.00 | 35.84 |
| ATOM | 2366 | CG | MET | 1731 | 31.068 | -13.379 | 4.975 | 1.00 | 45.50 |
| ATOM | 2367 | SD | MET | 1731 | 31.347 | -15.167 | 4.865 | 1.00 | 56.40 |
| ATOM | 2368 | CE | MET | 1731 | 32.106 | -15.263 | 3.217 | 1.00 | 56.88 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2369 | C | MET | 1731 | 29.916 | -10.928 | 6.102 | 1.00 | 27.79 |
| ATOM | 2370 | O | MET | 1731 | 29.755 | -10.345 | 5.041 | 1.00 | 30.68 |
| ATOM | 2371 | N | MET | 1732 | 28.915 | -11.203 | 6.932 | 1.00 | 28.02 |
| ATOM | 2373 | CA | MET | 1732 | 27.546 | -10.804 | 6.639 | 1.00 | 25.74 |
| ATOM | 2374 | CB | MET | 1732 | 26.598 | -11.317 | 7.718 | 1.00 | 24.94 |
| ATOM | 2375 | CG | MET | 1732 | 25.153 | -10.911 | 7.492 | 1.00 | 22.96 |
| ATOM | 2376 | SD | MET | 1732 | 24.008 | -11.593 | 8.684 | 1.00 | 24.39 |
| ATOM | 2377 | CE | MET | 1732 | 23.798 | -13.272 | 8.002 | 1.00 | 18.04 |
| ATOM | 2378 | C | MET | 1732 | 27.470 | -9.273 | 6.559 | 1.00 | 25.81 |
| ATOM | 2379 | O | MET | 1732 | 26.889 | -8.729 | 5.620 | 1.00 | 26.85 |
| ATOM | 2380 | N | MET | 1733 | 28.068 | -8.587 | 7.537 | 1.00 | 24.84 |
| ATOM | 2382 | CA | MET | 1733 | 28.092 | -7.124 | 7.545 | 1.00 | 25.27 |
| ATOM | 2383 | CB | MET | 1733 | 28.931 | -6.600 | 8.700 | 1.00 | 25.97 |
| ATOM | 2384 | CG | MET | 1733 | 28.342 | -6.769 | 10.058 | 1.00 | 28.69 |
| ATOM | 2385 | SD | MET | 1733 | 29.456 | -6.094 | 11.295 | 1.00 | 29.06 |
| ATOM | 2386 | CE | MET | 1733 | 28.927 | -7.051 | 12.693 | 1.00 | 28.07 |
| ATOM | 2387 | C | MET | 1733 | 28.741 | -6.628 | 6.270 | 1.00 | 26.97 |
| ATOM | 2388 | O | MET | 1733 | 28.192 | -5.771 | 5.581 | 1.00 | 28.37 |
| ATOM | 2389 | N | ARG | 1734 | 29.922 | -7.160 | 5.966 | 1.00 | 28.77 |
| ATOM | 2391 | CA | ARG | 1734 | 30.664 | -6.775 | 4.762 | 1.00 | 29.66 |
| ATOM | 2392 | CB | ARG | 1734 | 32.027 | -7.482 | 4.716 | 1.00 | 29.05 |
| ATOM | 2393 | CG | ARG | 1734 | 32.968 | -7.109 | 5.866 | 1.00 | 25.00 |
| ATOM | 2394 | CD | ARG | 1734 | 33.247 | -5.621 | 5.882 | 1.00 | 29.27 |
| ATOM | 2395 | NE | ARG | 1734 | 33.911 | -5.210 | 4.647 | 1.00 | 35.43 |
| ATOM | 2397 | CZ | ARG | 1734 | 35.233 | -5.220 | 4.466 | 1.00 | 38.24 |
| ATOM | 2398 | NH1 | ARG | 1734 | 36.054 | -5.601 | 5.445 | 1.00 | 36.47 |
| ATOM | 2401 | NH2 | ARG | 1734 | 35.732 | -4.907 | 3.277 | 1.00 | 38.57 |
| ATOM | 2404 | C | ARG | 1734 | 29.859 | -7.034 | 3.478 | 1.00 | 29.57 |
| ATOM | 2405 | O | ARG | 1734 | 29.920 | -6.242 | 2.538 | 1.00 | 29.55 |
| ATOM | 2406 | N | ASP | 1735 | 29.095 | -8.124 | 3.448 | 1.00 | 28.07 |
| ATOM | 2408 | CA | ASP | 1735 | 28.259 | -8.423 | 2.287 | 1.00 | 27.96 |
| ATOM | 2409 | CB | ASP | 1735 | 27.634 | -9.813 | 2.408 | 1.00 | 28.60 |
| ATOM | 2410 | CG | ASP | 1735 | 28.664 | -10.926 | 2.283 | 1.00 | 31.34 |
| ATOM | 2411 | OD1 | ASP | 1735 | 29.785 | -10.660 | 1.798 | 1.00 | 31.12 |
| ATOM | 2412 | OD2 | ASP | 1735 | 28.356 | -12.068 | 2.687 | 1.00 | 36.07 |
| ATOM | 2413 | C | ASP | 1735 | 27.159 | -7.368 | 2.155 | 1.00 | 27.24 |
| ATOM | 2414 | O | ASP | 1735 | 26.846 | -6.932 | 1.050 | 1.00 | 25.79 |
| ATOM | 2415 | N | CYS | 1736 | 26.590 | -6.951 | 3.288 | 1.00 | 26.53 |
| ATOM | 2417 | CA | CYS | 1736 | 25.547 | -5.930 | 3.314 | 1.00 | 24.35 |
| ATOM | 2418 | CB | CYS | 1736 | 24.968 | -5.765 | 4.731 | 1.00 | 22.01 |
| ATOM | 2419 | SG | CYS | 1736 | 23.885 | -7.101 | 5.281 | 1.00 | 21.52 |
| ATOM | 2420 | C | CYS | 1736 | 26.119 | -4.595 | 2.847 | 1.00 | 24.26 |
| ATOM | 2421 | O | CYS | 1736 | 25.386 | -3.725 | 2.368 | 1.00 | 24.19 |
| ATOM | 2422 | N | TRP | 1737 | 27.432 | -4.437 | 3.002 | 1.00 | 22.94 |
| ATOM | 2424 | CA | TRP | 1737 | 28.104 | -3.210 | 2.605 | 1.00 | 21.91 |
| ATOM | 2425 | CB | TRP | 1737 | 29.146 | -2.820 | 3.640 | 1.00 | 19.26 |
| ATOM | 2426 | CG | TRP | 1737 | 28.572 | -2.493 | 4.947 | 1.00 | 20.89 |
| ATOM | 2427 | CD2 | TRP | 1737 | 29.226 | -2.602 | 6.212 | 1.00 | 23.33 |
| ATOM | 2428 | CE2 | TRP | 1737 | 28.315 | -2.159 | 7.196 | 1.00 | 21.59 |
| ATOM | 2429 | CE3 | TRP | 1737 | 30.506 | -3.026 | 6.614 | 1.00 | 25.00 |
| ATOM | 2430 | CD1 | TRP | 1737 | 27.319 | -2.012 | 5.201 | 1.00 | 19.90 |
| ATOM | 2431 | NE1 | TRP | 1737 | 27.158 | -1.807 | 6.551 | 1.00 | 20.77 |
| ATOM | 2433 | CZ2 | TRP | 1737 | 28.641 | -2.127 | 8.563 | 1.00 | 19.89 |
| ATOM | 2434 | CZ3 | TRP | 1737 | 30.825 | -2.993 | 7.971 | 1.00 | 21.23 |

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|---|---|---|---|---|---|---|---|---|
| ATOM | 2435 | CH2 | TRP | 1737 | 29.896 | -2.543 | 8.927 | 1.00 | 21.09 |
| ATOM | 2436 | C | TRP | 1737 | 28.758 | -3.266 | 1.232 | 1.00 | 23.54 |
| ATOM | 2437 | O | TRP | 1737 | 29.653 | -2.477 | 0.939 | 1.00 | 24.68 |
| ATOM | 2438 | N | HIS | 1738 | 28.315 | -4.185 | 0.382 | 1.00 | 24.37 |
| ATOM | 2440 | CA | HIS | 1738 | 28.877 | -4.287 | -0.947 | 1.00 | 24.42 |
| ATOM | 2441 | CB | HIS | 1738 | 28.243 | -5.436 | -1.728 | 1.00 | 23.72 |
| ATOM | 2442 | CG | HIS | 1738 | 29.131 | -5.985 | -2.801 | 1.00 | 27.20 |
| ATOM | 2443 | CD2 | HIS | 1738 | 29.595 | -5.425 | -3.948 | 1.00 | 26.45 |
| ATOM | 2444 | ND1 | HIS | 1738 | 29.681 | -7.255 | -2.751 | 1.00 | 29.26 |
| ATOM | 2446 | CE1 | HIS | 1738 | 30.436 | -7.441 | -3.816 | 1.00 | 29.25 |
| ATOM | 2447 | NE2 | HIS | 1738 | 30.409 | -6.358 | -4.556 | 1.00 | 27.32 |
| ATOM | 2449 | C | HIS | 1738 | 28.716 | -2.970 | -1.713 | 1.00 | 25.82 |
| ATOM | 2450 | O | HIS | 1738 | 27.675 | -2.314 | -1.660 | 1.00 | 23.96 |
| ATOM | 2451 | N | ALA | 1739 | 29.802 | -2.564 | -2.362 | 1.00 | 26.27 |
| ATOM | 2453 | CA | ALA | 1739 | 29.825 | -1.346 | -3.158 | 1.00 | 25.46 |
| ATOM | 2454 | CB | ALA | 1739 | 31.186 | -1.180 | -3.789 | 1.00 | 25.70 |
| ATOM | 2455 | C | ALA | 1739 | 28.754 | -1.443 | -4.233 | 1.00 | 26.18 |
| ATOM | 2456 | O | ALA | 1739 | 28.116 | -0.455 | -4.574 | 1.00 | 29.14 |
| ATOM | 2457 | N | VAL | 1740 | 28.570 | -2.643 | -4.774 | 1.00 | 25.71 |
| ATOM | 2459 | CA | VAL | 1740 | 27.560 | -2.875 | -5.802 | 1.00 | 26.12 |
| ATOM | 2460 | CB | VAL | 1740 | 28.063 | -3.841 | -6.903 | 1.00 | 25.99 |
| ATOM | 2461 | CG1 | VAL | 1740 | 27.102 | -3.832 | -8.090 | 1.00 | 23.37 |
| ATOM | 2462 | CG2 | VAL | 1740 | 29.450 | -3.440 | -7.349 | 1.00 | 22.07 |
| ATOM | 2463 | C | VAL | 1740 | 26.247 | -3.400 | -5.191 | 1.00 | 25.43 |
| ATOM | 2464 | O | VAL | 1740 | 26.186 | -4.550 | -4.704 | 1.00 | 24.93 |
| ATOM | 2465 | N | PRO | 1741 | 25.170 | -2.585 | -5.265 | 1.00 | 24.20 |
| ATOM | 2466 | CD | PRO | 1741 | 25.151 | -1.277 | -5.953 | 1.00 | 18.88 |
| ATOM | 2467 | CA | PRO | 1741 | 23.838 | -2.914 | -4.734 | 1.00 | 25.28 |
| ATOM | 2468 | CB | PRO | 1741 | 22.953 | -1.788 | -5.294 | 1.00 | 22.75 |
| ATOM | 2469 | CG | PRO | 1741 | 23.903 | -0.632 | -5.398 | 1.00 | 20.99 |
| ATOM | 2470 | C | PRO | 1741 | 23.299 | -4.296 | -5.128 | 1.00 | 25.84 |
| ATOM | 2471 | O | PRO | 1741 | 22.787 | -5.036 | -4.280 | 1.00 | 25.99 |
| ATOM | 2472 | N | SER | 1742 | 23.425 | -4.642 | -6.407 | 1.00 | 26.48 |
| ATOM | 2474 | CA | SER | 1742 | 22.942 | -5.919 | -6.930 | 1.00 | 25.19 |
| ATOM | 2475 | CB | SER | 1742 | 23.151 | -5.992 | -8.440 | 1.00 | 25.68 |
| ATOM | 2476 | OG | SER | 1742 | 24.530 | -5.943 | -8.769 | 1.00 | 27.46 |
| ATOM | 2478 | C | SER | 1742 | 23.644 | -7.100 | -6.289 | 1.00 | 25.24 |
| ATOM | 2479 | O | SER | 1742 | 23.124 | -8.218 | -6.300 | 1.00 | 26.09 |
| ATOM | 2480 | N | GLN | 1743 | 24.826 | -6.851 | -5.731 | 1.00 | 23.88 |
| ATOM | 2482 | CA | GLN | 1743 | 25.590 | -7.917 | -5.118 | 1.00 | 24.44 |
| ATOM | 2483 | CB | GLN | 1743 | 27.069 | -7.733 | -5.437 | 1.00 | 27.26 |
| ATOM | 2484 | CG | GLN | 1743 | 27.344 | -7.784 | -6.940 | 1.00 | 27.39 |
| ATOM | 2485 | CD | GLN | 1743 | 26.803 | -9.047 | -7.581 | 1.00 | 26.46 |
| ATOM | 2486 | OE1 | GLN | 1743 | 27.325 | -10.136 | -7.339 | 1.00 | 25.80 |
| ATOM | 2487 | NE2 | GLN | 1743 | 25.760 | -8.914 | -8.393 | 1.00 | 27.42 |
| ATOM | 2490 | C | GLN | 1743 | 25.348 | -8.151 | -3.633 | 1.00 | 23.20 |
| ATOM | 2491 | O | GLN | 1743 | 25.810 | -9.147 | -3.083 | 1.00 | 22.90 |
| ATOM | 2492 | N | ARG | 1744 | 24.628 | -7.243 | -2.984 | 1.00 | 22.15 |
| ATOM | 2494 | CA | ARG | 1744 | 24.318 | -7.398 | -1.568 | 1.00 | 21.23 |
| ATOM | 2495 | CB | ARG | 1744 | 23.767 | -6.088 | -0.998 | 1.00 | 19.01 |
| ATOM | 2496 | CG | ARG | 1744 | 24.705 | -4.916 | -1.145 | 1.00 | 17.27 |
| ATOM | 2497 | CD | ARG | 1744 | 24.091 | -3.605 | -0.679 | 1.00 | 14.79 |
| ATOM | 2498 | NE | ARG | 1744 | 24.914 | -2.493 | -1.157 | 1.00 | 19.72 |
| ATOM | 2500 | CZ | ARG | 1744 | 24.482 | -1.258 | -1.391 | 1.00 | 19.23 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2501 | NH1 | ARG | 1744 | 23.201 | -0.931 | -1.201 | 1.00 | 15.90 |
| ATOM | 2504 | NH2 | ARG | 1744 | 25.343 | -0.343 | -1.821 | 1.00 | 19.43 |
| ATOM | 2507 | C | ARG | 1744 | 23.259 | -8.496 | -1.438 | 1.00 | 21.95 |
| ATOM | 2508 | O | ARG | 1744 | 22.585 | -8.827 | -2.415 | 1.00 | 25.34 |
| ATOM | 2509 | N | PRO | 1745 | 23.213 | -9.184 | -0.292 | 1.00 | 20.82 |
| ATOM | 2510 | CD | PRO | 1745 | 24.191 | -9.219 | 0.804 | 1.00 | 21.25 |
| ATOM | 2511 | CA | PRO | 1745 | 22.204 | -10.229 | -0.127 | 1.00 | 21.39 |
| ATOM | 2512 | CB | PRO | 1745 | 22.687 | -10.980 | 1.117 | 1.00 | 21.69 |
| ATOM | 2513 | CG | PRO | 1745 | 23.418 | -9.916 | 1.886 | 1.00 | 22.62 |
| ATOM | 2514 | C | PRO | 1745 | 20.833 | -9.585 | 0.102 | 1.00 | 22.15 |
| ATOM | 2515 | O | PRO | 1745 | 20.739 | -8.402 | 0.426 | 1.00 | 23.29 |
| ATOM | 2516 | N | THR | 1746 | 19.771 | -10.349 | -0.109 | 1.00 | 20.93 |
| ATOM | 2518 | CA | THR | 1746 | 18.440 | -9.827 | 0.107 | 1.00 | 19.90 |
| ATOM | 2519 | CB | THR | 1746 | 17.391 | -10.554 | -0.783 | 1.00 | 20.21 |
| ATOM | 2520 | OG1 | THR | 1746 | 17.484 | -11.974 | -0.584 | 1.00 | 22.03 |
| ATOM | 2522 | CG2 | THR | 1746 | 17.609 | -10.242 | -2.255 | 1.00 | 20.82 |
| ATOM | 2523 | C | THR | 1746 | 18.112 | -10.095 | 1.557 | 1.00 | 19.77 |
| ATOM | 2524 | O | THR | 1746 | 18.842 | -10.823 | 2.228 | 1.00 | 19.19 |
| ATOM | 2525 | N | PHE | 1747 | 17.010 | -9.526 | 2.045 | 1.00 | 23.46 |
| ATOM | 2527 | CA | PHE | 1747 | 16.582 | -9.770 | 3.422 | 1.00 | 21.64 |
| ATOM | 2528 | CB | PHE | 1747 | 15.473 | -8.794 | 3.827 | 1.00 | 18.89 |
| ATOM | 2529 | CG | PHE | 1747 | 15.987 | -7.445 | 4.262 | 1.00 | 17.45 |
| ATOM | 2530 | CD1 | PHE | 1747 | 16.757 | -7.317 | 5.417 | 1.00 | 17.65 |
| ATOM | 2531 | CD2 | PHE | 1747 | 15.712 | -6.303 | 3.516 | 1.00 | 15.37 |
| ATOM | 2532 | CE1 | PHE | 1747 | 17.242 | -6.073 | 5.819 | 1.00 | 16.17 |
| ATOM | 2533 | CE2 | PHE | 1747 | 16.189 | -5.056 | 3.907 | 1.00 | 14.53 |
| ATOM | 2534 | CZ | PHE | 1747 | 16.959 | -4.941 | 5.065 | 1.00 | 16.88 |
| ATOM | 2535 | C | PHE | 1747 | 16.118 | -11.227 | 3.522 | 1.00 | 23.18 |
| ATOM | 2536 | O | PHE | 1747 | 16.271 | -11.873 | 4.548 | 1.00 | 24.04 |
| ATOM | 2537 | N | LYS | 1748 | 15.570 | -11.745 | 2.432 | 1.00 | 24.13 |
| ATOM | 2539 | CA | LYS | 1748 | 15.137 | -13.132 | 2.385 | 1.00 | 26.35 |
| ATOM | 2540 | CB | LYS | 1748 | 14.502 | -13.424 | 1.024 | 1.00 | 27.52 |
| ATOM | 2541 | CG | LYS | 1748 | 14.034 | -14.849 | 0.836 | 1.00 | 33.88 |
| ATOM | 2542 | CD | LYS | 1748 | 13.598 | -15.062 | -0.600 | 1.00 | 41.83 |
| ATOM | 2543 | CE | LYS | 1748 | 13.190 | -16.506 | -0.881 | 1.00 | 50.05 |
| ATOM | 2544 | NZ | LYS | 1748 | 12.084 | -16.986 | 0.005 | 1.00 | 55.70 |
| ATOM | 2548 | C | LYS | 1748 | 16.359 | -14.037 | 2.636 | 1.00 | 27.50 |
| ATOM | 2549 | O | LYS | 1748 | 16.303 | -14.950 | 3.459 | 1.00 | 31.18 |
| ATOM | 2550 | N | GLN | 1749 | 17.467 | -13.761 | 1.949 | 1.00 | 27.24 |
| ATOM | 2552 | CA | GLN | 1749 | 18.699 | -14.529 | 2.122 | 1.00 | 27.03 |
| ATOM | 2553 | CB | GLN | 1749 | 19.797 | -14.039 | 1.169 | 1.00 | 31.80 |
| ATOM | 2554 | CG | GLN | 1749 | 19.501 | -14.196 | -0.323 | 1.00 | 38.57 |
| ATOM | 2555 | CD | GLN | 1749 | 20.460 | -13.385 | -1.209 | 1.00 | 39.93 |
| ATOM | 2556 | OE1 | GLN | 1749 | 20.025 | -12.535 | -1.974 | 1.00 | 39.90 |
| ATOM | 2557 | NE2 | GLN | 1749 | 21.768 | -13.620 | -1.068 | 1.00 | 40.23 |
| ATOM | 2560 | C | GLN | 1749 | 19.205 | -14.380 | 3.552 | 1.00 | 25.98 |
| ATOM | 2561 | O | GLN | 1749 | 19.533 | -15.371 | 4.198 | 1.00 | 27.18 |
| ATOM | 2562 | N | LEU | 1750 | 19.293 | -13.133 | 4.018 | 1.00 | 25.20 |
| ATOM | 2564 | CA | LEU | 1750 | 19.774 | -12.823 | 5.369 | 1.00 | 25.74 |
| ATOM | 2565 | CB | LEU | 1750 | 19.722 | -11.317 | 5.631 | 1.00 | 20.99 |
| ATOM | 2566 | CG | LEU | 1750 | 20.708 | -10.468 | 4.831 | 1.00 | 20.90 |
| ATOM | 2567 | CD1 | LEU | 1750 | 20.302 | -8.987 | 4.822 | 1.00 | 19.88 |
| ATOM | 2568 | CD2 | LEU | 1750 | 22.071 | -10.643 | 5.426 | 1.00 | 17.26 |
| ATOM | 2569 | C | LEU | 1750 | 18.985 | -13.555 | 6.441 | 1.00 | 27.10 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2570 | O | LEU | 1750 | 19.553 | -14.094 | 7.392 | 1.00 | 27.89 |
| ATOM | 2571 | N | VAL | 1751 | 17.672 | -13.598 | 6.265 | 1.00 | 29.40 |
| ATOM | 2573 | CA | VAL | 1751 | 16.798 | -14.262 | 7.210 | 1.00 | 26.80 |
| ATOM | 2574 | CB | VAL | 1751 | 15.324 | -14.030 | 6.843 | 1.00 | 26.94 |
| ATOM | 2575 | CG1 | VAL | 1751 | 14.429 | -14.941 | 7.657 | 1.00 | 29.93 |
| ATOM | 2576 | CG2 | VAL | 1751 | 14.941 | -12.575 | 7.117 | 1.00 | 24.10 |
| ATOM | 2577 | C | VAL | 1751 | 17.136 | -15.745 | 7.228 | 1.00 | 27.80 |
| ATOM | 2578 | O | VAL | 1751 | 17.223 | -16.359 | 8.285 | 1.00 | 26.77 |
| ATOM | 2579 | N | GLU | 1752 | 17.408 | -16.300 | 6.056 | 1.00 | 32.26 |
| ATOM | 2581 | CA | GLU | 1752 | 17.749 | -17.717 | 5.966 | 1.00 | 35.72 |
| ATOM | 2582 | CB | GLU | 1752 | 17.721 | -18.173 | 4.504 | 1.00 | 39.33 |
| ATOM | 2583 | CG | GLU | 1752 | 16.306 | -18.078 | 3.911 | 1.00 | 49.41 |
| ATOM | 2584 | CD | GLU | 1752 | 16.209 | -18.421 | 2.429 | 1.00 | 55.88 |
| ATOM | 2585 | OE1 | GLU | 1752 | 15.141 | -18.138 | 1.835 | 1.00 | 58.00 |
| ATOM | 2586 | OE2 | GLU | 1752 | 17.180 | -18.978 | 1.863 | 1.00 | 61.03 |
| ATOM | 2587 | C | GLU | 1752 | 19.093 | -18.002 | 6.635 | 1.00 | 34.59 |
| ATOM | 2588 | O | GLU | 1752 | 19.230 | -18.975 | 7.393 | 1.00 | 33.95 |
| ATOM | 2589 | N | ASP | 1753 | 20.057 | -17.114 | 6.401 | 1.00 | 34.38 |
| ATOM | 2591 | CA | ASP | 1753 | 21.393 | -17.235 | 6.977 | 1.00 | 32.81 |
| ATOM | 2592 | CB | ASP | 1753 | 22.338 | -16.227 | 6.334 | 1.00 | 31.57 |
| ATOM | 2593 | CG | ASP | 1753 | 22.628 | -16.556 | 4.888 | 1.00 | 33.68 |
| ATOM | 2594 | OD1 | ASP | 1753 | 22.573 | -17.755 | 4.536 | 1.00 | 35.14 |
| ATOM | 2595 | OD2 | ASP | 1753 | 22.914 | -15.624 | 4.104 | 1.00 | 34.44 |
| ATOM | 2596 | C | ASP | 1753 | 21.378 | -17.058 | 8.489 | 1.00 | 32.04 |
| ATOM | 2597 | O | ASP | 1753 | 21.997 | -17.837 | 9.214 | 1.00 | 31.21 |
| ATOM | 2598 | N | LEU | 1754 | 20.648 | -16.045 | 8.955 | 1.00 | 31.00 |
| ATOM | 2600 | CA | LEU | 1754 | 20.528 | -15.754 | 10.382 | 1.00 | 29.46 |
| ATOM | 2601 | CB | LEU | 1754 | 19.822 | -14.426 | 10.598 | 1.00 | 23.47 |
| ATOM | 2602 | CG | LEU | 1754 | 20.816 | -13.309 | 10.318 | 1.00 | 23.58 |
| ATOM | 2603 | CD1 | LEU | 1754 | 20.114 | -11.963 | 10.128 | 1.00 | 20.46 |
| ATOM | 2604 | CD2 | LEU | 1754 | 21.828 | -13.282 | 11.462 | 1.00 | 19.18 |
| ATOM | 2605 | C | LEU | 1754 | 19.806 | -16.866 | 11.110 | 1.00 | 31.84 |
| ATOM | 2606 | O | LEU | 1754 | 20.125 | -17.178 | 12.254 | 1.00 | 30.78 |
| ATOM | 2607 | N | ASP | 1755 | 18.832 | -17.471 | 10.445 | 1.00 | 34.03 |
| ATOM | 2609 | CA | ASP | 1755 | 18.116 | -18.578 | 11.044 | 1.00 | 35.22 |
| ATOM | 2610 | CB | ASP | 1755 | 16.973 | -19.027 | 10.148 | 1.00 | 38.40 |
| ATOM | 2611 | CG | ASP | 1755 | 16.159 | -20.119 | 10.779 | 1.00 | 41.85 |
| ATOM | 2612 | OD1 | ASP | 1755 | 15.560 | -19.866 | 11.841 | 1.00 | 47.90 |
| ATOM | 2613 | OD2 | ASP | 1755 | 16.142 | -21.241 | 10.238 | 1.00 | 46.67 |
| ATOM | 2614 | C | ASP | 1755 | 19.114 | -19.724 | 11.222 | 1.00 | 36.79 |
| ATOM | 2615 | O | ASP | 1755 | 19.114 | -20.411 | 12.250 | 1.00 | 38.33 |
| ATOM | 2616 | N | ARG | 1756 | 19.973 | -19.920 | 10.226 | 1.00 | 34.81 |
| ATOM | 2618 | CA | ARG | 1756 | 20.982 | -20.969 | 10.302 | 1.00 | 34.68 |
| ATOM | 2619 | CB | ARG | 1756 | 21.688 | -21.100 | 8.959 | 1.00 | 34.78 |
| ATOM | 2620 | CG | ARG | 1756 | 22.746 | -22.179 | 8.910 | 1.00 | 35.93 |
| ATOM | 2621 | CD | ARG | 1756 | 23.297 | -22.306 | 7.511 | 1.00 | 41.60 |
| ATOM | 2622 | NE | ARG | 1756 | 23.786 | -21.025 | 6.999 | 1.00 | 46.42 |
| ATOM | 2624 | CZ | ARG | 1756 | 24.889 | -20.419 | 7.427 | 1.00 | 48.38 |
| ATOM | 2625 | NH1 | ARG | 1756 | 25.637 | -20.976 | 8.381 | 1.00 | 48.10 |
| ATOM | 2628 | NH2 | ARG | 1756 | 25.236 | -19.242 | 6.909 | 1.00 | 46.62 |
| ATOM | 2631 | C | ARG | 1756 | 22.002 | -20.666 | 11.399 | 1.00 | 36.17 |
| ATOM | 2632 | O | ARG | 1756 | 22.372 | -21.541 | 12.177 | 1.00 | 38.33 |
| ATOM | 2633 | N | ILE | 1757 | 22.433 | -19.413 | 11.478 | 1.00 | 37.00 |
| ATOM | 2635 | CA | ILE | 1757 | 23.416 | -18.998 | 12.468 | 1.00 | 35.60 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2636 | CB | ILE | 1757 | 23.964 | -17.588 | 12.141 | 1.00 | 35.54 |
| ATOM | 2637 | CG2 | ILE | 1757 | 24.921 | -17.131 | 13.217 | 1.00 | 32.41 |
| ATOM | 2638 | CG1 | ILE | 1757 | 24.693 | -17.612 | 10.794 | 1.00 | 33.77 |
| ATOM | 2639 | CD1 | ILE | 1757 | 25.097 | -16.253 | 10.287 | 1.00 | 33.49 |
| ATOM | 2640 | C | ILE | 1757 | 22.866 | -19.048 | 13.891 | 1.00 | 37.28 |
| ATOM | 2641 | O | ILE | 1757 | 23.531 | -19.556 | 14.779 | 1.00 | 38.42 |
| ATOM | 2642 | N | VAL | 1758 | 21.634 | -18.585 | 14.088 | 1.00 | 39.19 |
| ATOM | 2644 | CA | VAL | 1758 | 21.016 | -18.584 | 15.421 | 1.00 | 39.84 |
| ATOM | 2645 | CB | VAL | 1758 | 19.560 | -18.017 | 15.403 | 1.00 | 37.62 |
| ATOM | 2646 | CG1 | VAL | 1758 | 18.918 | -18.144 | 16.773 | 1.00 | 38.30 |
| ATOM | 2647 | CG2 | VAL | 1758 | 19.560 | -16.560 | 15.009 | 1.00 | 39.62 |
| ATOM | 2648 | C | VAL | 1758 | 20.983 | -19.997 | 15.988 | 1.00 | 41.98 |
| ATOM | 2649 | O | VAL | 1758 | 21.380 | -20.229 | 17.128 | 1.00 | 43.36 |
| ATOM | 2650 | N | ALA | 1759 | 20.501 | -20.932 | 15.182 | 1.00 | 43.31 |
| ATOM | 2652 | CA | ALA | 1759 | 20.418 | -22.325 | 15.589 | 1.00 | 44.00 |
| ATOM | 2653 | CB | ALA | 1759 | 19.836 | -23.150 | 14.459 | 1.00 | 44.52 |
| ATOM | 2654 | C | ALA | 1759 | 21.784 | -22.867 | 15.976 | 1.00 | 45.98 |
| ATOM | 2655 | O | ALA | 1759 | 21.894 | -23.725 | 16.841 | 1.00 | 48.78 |
| ATOM | 2656 | N | LEU | 1760 | 22.823 | -22.375 | 15.319 | 1.00 | 48.93 |
| ATOM | 2658 | CA | LEU | 1760 | 24.175 | -22.831 | 15.592 | 1.00 | 51.47 |
| ATOM | 2659 | CB | LEU | 1760 | 24.954 | -22.900 | 14.280 | 1.00 | 53.63 |
| ATOM | 2660 | CG | LEU | 1760 | 24.284 | -23.864 | 13.295 | 1.00 | 57.84 |
| ATOM | 2661 | CD1 | LEU | 1760 | 24.993 | -23.847 | 11.948 | 1.00 | 61.83 |
| ATOM | 2662 | CD2 | LEU | 1760 | 24.260 | -25.277 | 13.886 | 1.00 | 58.57 |
| ATOM | 2663 | C | LEU | 1760 | 24.911 | -21.965 | 16.607 | 1.00 | 53.60 |
| ATOM | 2664 | O | LEU | 1760 | 26.078 | -22.214 | 16.919 | 1.00 | 54.00 |
| ATOM | 2665 | N | THR | 1761 | 24.222 | -20.963 | 17.141 | 1.00 | 55.77 |
| ATOM | 2667 | CA | THR | 1761 | 24.820 | -20.060 | 18.111 | 1.00 | 56.64 |
| ATOM | 2668 | CB | THR | 1761 | 24.250 | -18.627 | 17.979 | 1.00 | 55.76 |
| ATOM | 2669 | OG1 | THR | 1761 | 24.444 | -18.154 | 16.644 | 1.00 | 56.20 |
| ATOM | 2671 | CG2 | THR | 1761 | 24.962 | -17.680 | 18.917 | 1.00 | 55.25 |
| ATOM | 2672 | C | THR | 1761 | 24.636 | -20.548 | 19.539 | 1.00 | 58.16 |
| ATOM | 2673 | O | THR | 1761 | 23.566 | -21.021 | 19.919 | 1.00 | 56.85 |
| ATOM | 2674 | N | SER | 1762 | 25.706 | -20.436 | 20.318 | 1.00 | 61.74 |
| ATOM | 2676 | CA | SER | 1762 | 25.706 | -20.833 | 21.717 | 1.00 | 64.50 |
| ATOM | 2677 | CB | SER | 1762 | 27.155 | -20.979 | 22.205 | 1.00 | 68.82 |
| ATOM | 2678 | OG | SER | 1762 | 27.232 | -21.544 | 23.508 | 1.00 | 73.15 |
| ATOM | 2680 | C | SER | 1762 | 24.965 | -19.775 | 22.547 | 1.00 | 63.87 |
| ATOM | 2681 | O | SER | 1762 | 25.080 | -18.563 | 22.296 | 1.00 | 63.22 |
| ATOM | 3420 | PA | PCP | 400 | 62.748 | 10.301 | 7.817 | 1.00 | 90.90 |
| ATOM | 3421 | O1A | PCP | 400 | 62.509 | 10.036 | 9.280 | 1.00 | 92.35 |
| ATOM | 3422 | O2A | PCP | 400 | 61.832 | 11.180 | 7.038 | 1.00 | 90.49 |
| ATOM | 3423 | O5* | PCP | 400 | 62.744 | 8.904 | 7.142 | 1.00 | 83.57 |
| ATOM | 3424 | PB | PCP | 400 | 65.226 | 11.946 | 8.294 | 1.00 | 101.51 |
| ATOM | 3425 | O1B | PCP | 400 | 65.246 | 13.015 | 7.264 | 1.00 | 102.85 |
| ATOM | 3426 | O2B | PCP | 400 | 66.527 | 11.458 | 8.830 | 1.00 | 99.88 |
| ATOM | 3427 | O3A | PCP | 400 | 64.334 | 10.725 | 7.584 | 1.00 | 96.64 |
| ATOM | 3428 | C3B | PCP | 400 | 64.345 | 12.502 | 9.635 | 1.00 | 102.94 |
| ATOM | 3429 | C5* | PCP | 400 | 62.337 | 8.684 | 5.839 | 1.00 | 71.21 |
| ATOM | 3430 | C4* | PCP | 400 | 62.479 | 7.204 | 5.587 | 1.00 | 64.48 |
| ATOM | 3431 | O4* | PCP | 400 | 63.713 | 6.745 | 6.169 | 1.00 | 60.91 |
| ATOM | 3432 | C1* | PCP | 400 | 63.394 | 5.459 | 6.680 | 1.00 | 54.96 |
| ATOM | 3433 | N9 | PCP | 400 | 64.326 | 5.101 | 7.712 | 1.00 | 47.26 |
| ATOM | 3434 | C4 | PCP | 400 | 65.017 | 3.903 | 7.840 | 1.00 | 46.24 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3435 | N3 | PCP | 400 | 64.926 | 2.770 | 7.062 | 1.00 | 41.02 |
| ATOM | 3436 | C2 | PCP | 400 | 65.802 | 1.878 | 7.531 | 1.00 | 40.72 |
| ATOM | 3437 | N1 | PCP | 400 | 66.674 | 1.917 | 8.558 | 1.00 | 37.37 |
| ATOM | 3438 | C6 | PCP | 400 | 66.735 | 3.028 | 9.305 | 1.00 | 40.23 |
| ATOM | 3439 | N6 | PCP | 400 | 67.573 | 3.134 | 10.333 | 1.00 | 33.92 |
| ATOM | 3442 | C5 | PCP | 400 | 65.862 | 4.091 | 8.937 | 1.00 | 44.12 |
| ATOM | 3443 | N7 | PCP | 400 | 65.674 | 5.361 | 9.472 | 1.00 | 45.15 |
| ATOM | 3444 | C8 | PCP | 400 | 64.761 | 5.894 | 8.702 | 1.00 | 44.83 |
| ATOM | 3445 | C2* | PCP | 400 | 61.986 | 5.500 | 7.254 | 1.00 | 57.63 |
| ATOM | 3446 | O2* | PCP | 400 | 61.454 | 4.153 | 7.211 | 1.00 | 56.45 |
| ATOM | 3448 | C3* | PCP | 400 | 61.328 | 6.402 | 6.245 | 1.00 | 61.31 |
| ATOM | 3449 | O3* | PCP | 400 | 60.689 | 5.644 | 5.206 | 1.00 | 64.65 |
| ATOM | 3451 | PA | PCP | 401 | 9.366 | 9.801 | 17.743 | 0.50 | 74.43 |
| ATOM | 3452 | O1A | PCP | 401 | 9.463 | 8.736 | 16.709 | 0.50 | 75.37 |
| ATOM | 3453 | O2A | PCP | 401 | 10.330 | 10.926 | 17.699 | 0.50 | 75.86 |
| ATOM | 3454 | O5* | PCP | 401 | 9.427 | 9.108 | 19.186 | 0.50 | 67.44 |
| ATOM | 3455 | PB | PCP | 401 | 6.878 | 10.679 | 16.547 | 0.50 | 82.27 |
| ATOM | 3456 | O1B | PCP | 401 | 6.223 | 11.982 | 16.778 | 0.50 | 82.91 |
| ATOM | 3457 | O2B | PCP | 401 | 6.020 | 9.486 | 16.408 | 0.50 | 82.70 |
| ATOM | 3458 | O3A | PCP | 401 | 7.868 | 10.423 | 17.814 | 0.50 | 78.30 |
| ATOM | 3459 | C3B | PCP | 401 | 7.790 | 10.845 | 15.159 | 0.50 | 82.50 |
| ATOM | 3460 | C5* | PCP | 401 | 10.184 | 9.593 | 20.275 | 0.50 | 54.44 |
| ATOM | 3461 | C4* | PCP | 401 | 10.228 | 8.637 | 21.442 | 0.50 | 45.38 |
| ATOM | 3462 | O4* | PCP | 401 | 9.032 | 7.855 | 21.412 | 0.50 | 39.40 |
| ATOM | 3463 | C1* | PCP | 401 | 9.397 | 6.509 | 21.641 | 0.50 | 35.00 |
| ATOM | 3464 | N9 | PCP | 401 | 8.386 | 5.627 | 21.044 | 0.50 | 27.91 |
| ATOM | 3465 | C4 | PCP | 401 | 7.790 | 4.469 | 21.564 | 0.50 | 23.36 |
| ATOM | 3466 | N3 | PCP | 401 | 7.982 | 3.849 | 22.732 | 0.50 | 22.33 |
| ATOM | 3467 | C2 | PCP | 401 | 7.239 | 2.768 | 22.838 | 0.50 | 20.26 |
| ATOM | 3468 | N1 | PCP | 401 | 6.382 | 2.251 | 22.003 | 0.50 | 17.29 |
| ATOM | 3469 | C6 | PCP | 401 | 6.202 | 2.877 | 20.856 | 0.50 | 19.35 |
| ATOM | 3470 | N6 | PCP | 401 | 5.327 | 2.415 | 19.975 | 0.50 | 16.87 |
| ATOM | 3473 | C5 | PCP | 401 | 6.932 | 4.038 | 20.603 | 0.50 | 21.72 |
| ATOM | 3474 | N7 | PCP | 401 | 6.983 | 4.880 | 19.507 | 0.50 | 24.59 |
| ATOM | 3475 | C8 | PCP | 401 | 7.847 | 5.786 | 19.832 | 0.50 | 24.26 |
| ATOM | 3476 | C2* | PCP | 401 | 10.762 | 6.409 | 20.931 | 0.50 | 39.01 |
| ATOM | 3477 | O2* | PCP | 401 | 11.609 | 5.326 | 21.412 | 0.50 | 43.88 |
| ATOM | 3479 | C3* | PCP | 401 | 11.396 | 7.674 | 21.373 | 0.50 | 42.14 |
| ATOM | 3480 | O3* | PCP | 401 | 11.918 | 7.515 | 22.681 | 0.50 | 44.21 |
| ATOM | 3482 | N | SER | 461 | 78.844 | 26.057 | 14.057 | 1.00 | 43.87 |
| ATOM | 3484 | CA | SER | 461 | 79.399 | 24.884 | 13.385 | 1.00 | 43.50 |
| ATOM | 3485 | CB | SER | 461 | 78.488 | 23.655 | 13.616 | 1.00 | 39.99 |
| ATOM | 3486 | C | SER | 461 | 79.572 | 25.181 | 11.888 | 1.00 | 42.14 |
| ATOM | 3487 | O | SER | 461 | 79.473 | 24.292 | 11.038 | 1.00 | 40.29 |
| ATOM | 3488 | N | GLU | 462 | 79.883 | 26.441 | 11.594 | 1.00 | 43.19 |
| ATOM | 3490 | CA | GLU | 462 | 80.061 | 26.951 | 10.233 | 1.00 | 42.77 |
| ATOM | 3491 | CB | GLU | 462 | 80.303 | 28.446 | 10.250 | 1.00 | 47.75 |
| ATOM | 3492 | CG | GLU | 462 | 79.209 | 29.301 | 10.860 | 1.00 | 60.57 |
| ATOM | 3493 | CD | GLU | 462 | 79.647 | 30.752 | 11.061 | 1.00 | 67.56 |
| ATOM | 3494 | OE1 | GLU | 462 | 80.866 | 31.016 | 10.994 | 1.00 | 67.47 |
| ATOM | 3495 | OE2 | GLU | 462 | 78.764 | 31.611 | 11.296 | 1.00 | 72.32 |
| ATOM | 3496 | C | GLU | 462 | 81.207 | 26.357 | 9.457 | 1.00 | 39.55 |
| ATOM | 3497 | O | GLU | 462 | 81.051 | 26.032 | 8.292 | 1.00 | 38.74 |
| ATOM | 3498 | N | TYR | 463 | 82.375 | 26.299 | 10.091 | 1.00 | 36.47 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3500 | CA | TYR | 463 | 83.567 | 25.806 | 9.420 | 1.00 | 34.19 |
| ATOM | 3501 | CB | TYR | 463 | 84.702 | 26.828 | 9.505 | 1.00 | 35.55 |
| ATOM | 3502 | CG | TYR | 463 | 84.393 | 28.059 | 8.675 | 1.00 | 42.11 |
| ATOM | 3503 | CD1 | TYR | 463 | 84.004 | 29.264 | 9.283 | 1.00 | 43.15 |
| ATOM | 3504 | CE1 | TYR | 463 | 83.619 | 30.361 | 8.513 | 1.00 | 42.40 |
| ATOM | 3505 | CD2 | TYR | 463 | 84.395 | 27.990 | 7.280 | 1.00 | 39.78 |
| ATOM | 3506 | CE2 | TYR | 463 | 84.012 | 29.078 | 6.509 | 1.00 | 39.04 |
| ATOM | 3507 | CZ | TYR | 463 | 83.625 | 30.256 | 7.129 | 1.00 | 39.86 |
| ATOM | 3508 | OH | TYR | 463 | 83.260 | 31.330 | 6.366 | 1.00 | 42.58 |
| ATOM | 3510 | C | TYR | 463 | 84.055 | 24.434 | 9.800 | 1.00 | 33.28 |
| ATOM | 3511 | O | TYR | 463 | 84.739 | 23.781 | 9.005 | 1.00 | 33.47 |
| ATOM | 3512 | N | GLU | 464 | 83.695 | 23.976 | 10.993 | 1.00 | 34.42 |
| ATOM | 3514 | CA | GLU | 464 | 84.117 | 22.660 | 11.444 | 1.00 | 36.38 |
| ATOM | 3515 | CB | GLU | 464 | 85.618 | 22.663 | 11.750 | 1.00 | 40.90 |
| ATOM | 3516 | CG | GLU | 464 | 86.041 | 23.755 | 12.729 | 1.00 | 46.29 |
| ATOM | 3517 | CD | GLU | 464 | 87.548 | 23.810 | 12.943 | 1.00 | 51.33 |
| ATOM | 3518 | OE1 | GLU | 464 | 87.970 | 24.247 | 14.038 | 1.00 | 54.49 |
| ATOM | 3519 | OE2 | GLU | 464 | 88.312 | 23.430 | 12.025 | 1.00 | 53.18 |
| ATOM | 3520 | C | GLU | 464 | 83.374 | 22.224 | 12.678 | 1.00 | 35.64 |
| ATOM | 3521 | O | GLU | 464 | 83.111 | 23.052 | 13.555 | 1.00 | 37.40 |
| ATOM | 3522 | N | LEU | 465 | 82.962 | 20.955 | 12.711 | 1.00 | 34.21 |
| ATOM | 3524 | CA | LEU | 465 | 82.267 | 20.429 | 13.887 | 1.00 | 34.92 |
| ATOM | 3525 | CB | LEU | 465 | 81.285 | 19.300 | 13.542 | 1.00 | 31.30 |
| ATOM | 3526 | CG | LEU | 465 | 80.272 | 19.381 | 12.405 | 1.00 | 32.22 |
| ATOM | 3527 | CD1 | LEU | 465 | 79.152 | 18.407 | 12.720 | 1.00 | 21.95 |
| ATOM | 3528 | CD2 | LEU | 465 | 79.738 | 20.802 | 12.212 | 1.00 | 29.75 |
| ATOM | 3529 | C | LEU | 465 | 83.326 | 19.855 | 14.814 | 1.00 | 36.17 |
| ATOM | 3530 | O | LEU | 465 | 84.473 | 19.621 | 14.400 | 1.00 | 35.80 |
| ATOM | 3531 | N | PRO | 466 | 82.970 | 19.629 | 16.083 | 1.00 | 36.20 |
| ATOM | 3532 | CD | PRO | 466 | 81.722 | 20.018 | 16.758 | 1.00 | 38.17 |
| ATOM | 3533 | CA | PRO | 466 | 83.925 | 19.072 | 17.037 | 1.00 | 36.06 |
| ATOM | 3534 | CB | PRO | 466 | 83.132 | 19.035 | 18.333 | 1.00 | 35.57 |
| ATOM | 3535 | CG | PRO | 466 | 82.185 | 20.194 | 18.171 | 1.00 | 38.67 |
| ATOM | 3536 | C | PRO | 466 | 84.294 | 17.666 | 16.605 | 1.00 | 37.06 |
| ATOM | 3537 | O | PRO | 466 | 83.498 | 16.959 | 15.979 | 1.00 | 34.50 |
| ATOM | 3538 | N | GLU | 467 | 85.504 | 17.258 | 16.936 | 1.00 | 39.97 |
| ATOM | 3540 | CA | GLU | 467 | 85.951 | 15.932 | 16.587 | 1.00 | 44.69 |
| ATOM | 3541 | CB | GLU | 467 | 87.412 | 15.985 | 16.151 | 1.00 | 50.43 |
| ATOM | 3542 | CG | GLU | 467 | 87.902 | 14.695 | 15.518 | 1.00 | 60.27 |
| ATOM | 3543 | CD | GLU | 467 | 89.321 | 14.796 | 14.986 | 1.00 | 65.75 |
| ATOM | 3544 | OE1 | GLU | 467 | 90.024 | 15.804 | 15.269 | 1.00 | 64.40 |
| ATOM | 3545 | OE2 | GLU | 467 | 89.726 | 13.850 | 14.275 | 1.00 | 71.13 |
| ATOM | 3546 | C | GLU | 467 | 85.775 | 15.002 | 17.783 | 1.00 | 43.30 |
| ATOM | 3547 | O | GLU | 467 | 85.888 | 15.428 | 18.936 | 1.00 | 43.26 |
| ATOM | 3548 | N | ASP | 468 | 85.433 | 13.750 | 17.504 | 1.00 | 43.09 |
| ATOM | 3550 | CA | ASP | 468 | 85.254 | 12.739 | 18.545 | 1.00 | 44.15 |
| ATOM | 3551 | CB | ASP | 468 | 83.785 | 12.614 | 18.979 | 1.00 | 44.54 |
| ATOM | 3552 | CG | ASP | 468 | 83.574 | 11.562 | 20.072 | 1.00 | 41.84 |
| ATOM | 3553 | OD1 | ASP | 468 | 82.405 | 11.244 | 20.368 | 1.00 | 39.81 |
| ATOM | 3554 | OD2 | ASP | 468 | 84.570 | 11.057 | 20.636 | 1.00 | 42.92 |
| ATOM | 3555 | C | ASP | 468 | 85.746 | 11.422 | 17.970 | 1.00 | 44.66 |
| ATOM | 3556 | O | ASP | 468 | 84.982 | 10.663 | 17.368 | 1.00 | 44.56 |
| ATOM | 3557 | N | PRO | 469 | 87.034 | 11.126 | 18.176 | 1.00 | 44.56 |
| ATOM | 3558 | CD | PRO | 469 | 87.953 | 11.959 | 18.971 | 1.00 | 45.43 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3559 | CA | PRO | 469 | 87.707 | 9.916 | 17.707 | 1.00 | 43.90 |
| ATOM | 3560 | CB | PRO | 469 | 89.024 | 9.959 | 18.476 | 1.00 | 45.66 |
| ATOM | 3561 | CG | PRO | 469 | 89.300 | 11.438 | 18.547 | 1.00 | 44.89 |
| ATOM | 3562 | C | PRO | 469 | 86.934 | 8.627 | 17.971 | 1.00 | 42.60 |
| ATOM | 3563 | O | PRO | 469 | 86.935 | 7.730 | 17.139 | 1.00 | 41.35 |
| ATOM | 3564 | N | ARG | 470 | 86.229 | 8.569 | 19.096 | 1.00 | 43.25 |
| ATOM | 3566 | CA | ARG | 470 | 85.460 | 7.380 | 19.470 | 1.00 | 44.81 |
| ATOM | 3567 | CB | ARG | 470 | 84.722 | 7.612 | 20.789 | 1.00 | 48.36 |
| ATOM | 3568 | CG | ARG | 470 | 85.579 | 8.201 | 21.889 | 1.00 | 53.41 |
| ATOM | 3569 | CD | ARG | 470 | 84.764 | 8.458 | 23.138 | 1.00 | 55.42 |
| ATOM | 3570 | NE | ARG | 470 | 83.581 | 9.261 | 22.861 | 1.00 | 58.57 |
| ATOM | 3572 | CZ | ARG | 470 | 82.748 | 9.712 | 23.791 | 1.00 | 62.24 |
| ATOM | 3573 | NH1 | ARG | 470 | 82.972 | 9.445 | 25.077 | 1.00 | 64.57 |
| ATOM | 3576 | NH2 | ARG | 470 | 81.670 | 10.398 | 23.436 | 1.00 | 63.66 |
| ATOM | 3579 | C | ARG | 470 | 84.439 | 6.924 | 18.437 | 1.00 | 43.69 |
| ATOM | 3580 | O | ARG | 470 | 84.166 | 5.735 | 18.313 | 1.00 | 45.68 |
| ATOM | 3581 | N | TRP | 471 | 83.879 | 7.866 | 17.693 | 1.00 | 42.41 |
| ATOM | 3583 | CA | TRP | 471 | 82.851 | 7.534 | 16.720 | 1.00 | 38.92 |
| ATOM | 3584 | CB | TRP | 471 | 81.577 | 8.268 | 17.095 | 1.00 | 35.80 |
| ATOM | 3585 | CG | TRP | 471 | 80.967 | 7.741 | 18.335 | 1.00 | 37.13 |
| ATOM | 3586 | CD2 | TRP | 471 | 80.158 | 6.569 | 18.443 | 1.00 | 37.26 |
| ATOM | 3587 | CE2 | TRP | 471 | 79.723 | 6.483 | 19.785 | 1.00 | 38.20 |
| ATOM | 3588 | CE3 | TRP | 471 | 79.748 | 5.582 | 17.530 | 1.00 | 35.59 |
| ATOM | 3589 | CD1 | TRP | 471 | 81.010 | 8.300 | 19.584 | 1.00 | 36.42 |
| ATOM | 3590 | NE1 | TRP | 471 | 80.260 | 7.553 | 20.462 | 1.00 | 35.89 |
| ATOM | 3592 | CZ2 | TRP | 471 | 78.896 | 5.454 | 20.239 | 1.00 | 36.18 |
| ATOM | 3593 | CZ3 | TRP | 471 | 78.934 | 4.561 | 17.978 | 1.00 | 32.81 |
| ATOM | 3594 | CH2 | TRP | 471 | 78.514 | 4.505 | 19.321 | 1.00 | 34.82 |
| ATOM | 3595 | C | TRP | 471 | 83.175 | 7.845 | 15.277 | 1.00 | 39.77 |
| ATOM | 3596 | O | TRP | 471 | 82.478 | 7.391 | 14.362 | 1.00 | 39.56 |
| ATOM | 3597 | N | GLU | 472 | 84.224 | 8.628 | 15.075 | 1.00 | 39.37 |
| ATOM | 3599 | CA | GLU | 472 | 84.605 | 9.043 | 13.739 | 1.00 | 38.42 |
| ATOM | 3600 | CB | GLU | 472 | 85.794 | 9.994 | 13.812 | 1.00 | 37.11 |
| ATOM | 3601 | CG | GLU | 472 | 85.958 | 10.849 | 12.582 | 1.00 | 34.11 |
| ATOM | 3602 | CD | GLU | 472 | 84.772 | 11.757 | 12.338 | 1.00 | 34.03 |
| ATOM | 3603 | OE1 | GLU | 472 | 84.260 | 12.348 | 13.317 | 1.00 | 31.87 |
| ATOM | 3604 | OE2 | GLU | 472 | 84.367 | 11.885 | 11.163 | 1.00 | 32.11 |
| ATOM | 3605 | C | GLU | 472 | 84.910 | 7.901 | 12.791 | 1.00 | 39.78 |
| ATOM | 3606 | O | GLU | 472 | 85.656 | 6.975 | 13.128 | 1.00 | 41.64 |
| ATOM | 3607 | N | LEU | 473 | 84.303 | 7.958 | 11.610 | 1.00 | 37.71 |
| ATOM | 3609 | CA | LEU | 473 | 84.538 | 6.957 | 10.590 | 1.00 | 36.94 |
| ATOM | 3610 | CB | LEU | 473 | 83.258 | 6.196 | 10.265 | 1.00 | 35.38 |
| ATOM | 3611 | CG | LEU | 473 | 83.438 | 5.065 | 9.236 | 1.00 | 37.67 |
| ATOM | 3612 | CD1 | LEU | 473 | 84.070 | 3.845 | 9.903 | 1.00 | 37.28 |
| ATOM | 3613 | CD2 | LEU | 473 | 82.106 | 4.687 | 8.598 | 1.00 | 37.87 |
| ATOM | 3614 | C | LEU | 473 | 85.035 | 7.664 | 9.330 | 1.00 | 39.31 |
| ATOM | 3615 | O | LEU | 473 | 84.484 | 8.697 | 8.938 | 1.00 | 40.55 |
| ATOM | 3616 | N | PRO | 474 | 86.140 | 7.164 | 8.732 | 1.00 | 39.20 |
| ATOM | 3617 | CD | PRO | 474 | 87.052 | 6.170 | 9.327 | 1.00 | 37.83 |
| ATOM | 3618 | CA | PRO | 474 | 86.735 | 7.716 | 7.513 | 1.00 | 38.53 |
| ATOM | 3619 | CB | PRO | 474 | 87.914 | 6.777 | 7.282 | 1.00 | 37.16 |
| ATOM | 3620 | CG | PRO | 474 | 88.355 | 6.488 | 8.644 | 1.00 | 34.42 |
| ATOM | 3621 | C | PRO | 474 | 85.733 | 7.607 | 6.370 | 1.00 | 40.25 |
| ATOM | 3622 | O | PRO | 474 | 85.220 | 6.523 | 6.098 | 1.00 | 40.70 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3623 | N | ARG | 475 | 85.492 | 8.723 | 5.685 | 1.00 | 41.09 |
| ATOM | 3625 | CA | ARG | 475 | 84.534 | 8.746 | 4.590 | 1.00 | 42.26 |
| ATOM | 3626 | CB | ARG | 475 | 84.487 | 10.132 | 3.948 | 1.00 | 39.19 |
| ATOM | 3627 | CG | ARG | 475 | 83.957 | 11.199 | 4.876 | 1.00 | 35.19 |
| ATOM | 3628 | CD | ARG | 475 | 84.074 | 12.593 | 4.301 | 1.00 | 30.76 |
| ATOM | 3629 | NE | ARG | 475 | 83.796 | 13.567 | 5.345 | 1.00 | 22.86 |
| ATOM | 3631 | CZ | ARG | 475 | 82.581 | 13.898 | 5.748 | 1.00 | 21.99 |
| ATOM | 3632 | NH1 | ARG | 475 | 81.529 | 13.350 | 5.165 | 1.00 | 23.39 |
| ATOM | 3635 | NH2 | ARG | 475 | 82.412 | 14.662 | 6.813 | 1.00 | 22.55 |
| ATOM | 3638 | C | ARG | 475 | 84.838 | 7.692 | 3.538 | 1.00 | 45.38 |
| ATOM | 3639 | O | ARG | 475 | 83.927 | 7.182 | 2.892 | 1.00 | 47.15 |
| ATOM | 3640 | N | ASP | 476 | 86.106 | 7.319 | 3.390 | 1.00 | 47.13 |
| ATOM | 3642 | CA | ASP | 476 | 86.461 | 6.325 | 2.387 | 1.00 | 51.33 |
| ATOM | 3643 | CB | ASP | 476 | 87.973 | 6.294 | 2.134 | 1.00 | 55.23 |
| ATOM | 3644 | CG | ASP | 476 | 88.768 | 5.841 | 3.340 | 1.00 | 61.16 |
| ATOM | 3645 | OD1 | ASP | 476 | 88.863 | 4.617 | 3.573 | 1.00 | 65.55 |
| ATOM | 3646 | OD2 | ASP | 476 | 89.331 | 6.713 | 4.036 | 1.00 | 65.78 |
| ATOM | 3647 | C | ASP | 476 | 85.932 | 4.940 | 2.746 | 1.00 | 52.35 |
| ATOM | 3648 | O | ASP | 476 | 85.815 | 4.063 | 1.885 | 1.00 | 55.49 |
| ATOM | 3649 | N | ARG | 477 | 85.609 | 4.752 | 4.021 | 1.00 | 50.77 |
| ATOM | 3651 | CA | ARG | 477 | 85.080 | 3.482 | 4.508 | 1.00 | 48.65 |
| ATOM | 3652 | CB | ARG | 477 | 85.612 | 3.208 | 5.908 | 1.00 | 50.02 |
| ATOM | 3653 | CG | ARG | 477 | 87.067 | 2.799 | 5.881 | 1.00 | 55.33 |
| ATOM | 3654 | CD | ARG | 477 | 87.760 | 3.030 | 7.201 | 1.00 | 60.38 |
| ATOM | 3655 | NE | ARG | 477 | 87.238 | 2.207 | 8.285 | 1.00 | 64.36 |
| ATOM | 3657 | CZ | ARG | 477 | 87.748 | 2.203 | 9.513 | 1.00 | 69.16 |
| ATOM | 3658 | NH1 | ARG | 477 | 88.794 | 2.968 | 9.814 | 1.00 | 70.73 |
| ATOM | 3661 | NH2 | ARG | 477 | 87.190 | 1.459 | 10.459 | 1.00 | 71.59 |
| ATOM | 3664 | C | ARG | 477 | 83.546 | 3.414 | 4.484 | 1.00 | 46.25 |
| ATOM | 3665 | O | ARG | 477 | 82.957 | 2.481 | 5.013 | 1.00 | 46.36 |
| ATOM | 3666 | N | LEU | 478 | 82.913 | 4.372 | 3.815 | 1.00 | 42.23 |
| ATOM | 3668 | CA | LEU | 478 | 81.464 | 4.418 | 3.743 | 1.00 | 38.89 |
| ATOM | 3669 | CB | LEU | 478 | 80.938 | 5.537 | 4.657 | 1.00 | 37.17 |
| ATOM | 3670 | CG | LEU | 478 | 79.418 | 5.733 | 4.678 | 1.00 | 34.13 |
| ATOM | 3671 | CD1 | LEU | 478 | 78.777 | 4.723 | 5.609 | 1.00 | 32.24 |
| ATOM | 3672 | CD2 | LEU | 478 | 79.074 | 7.133 | 5.101 | 1.00 | 33.15 |
| ATOM | 3673 | C | LEU | 478 | 81.059 | 4.697 | 2.303 | 1.00 | 38.34 |
| ATOM | 3674 | O | LEU | 478 | 81.515 | 5.671 | 1.711 | 1.00 | 40.88 |
| ATOM | 3675 | N | VAL | 479 | 80.208 | 3.850 | 1.738 | 1.00 | 37.34 |
| ATOM | 3677 | CA | VAL | 479 | 79.763 | 4.042 | 0.364 | 1.00 | 37.61 |
| ATOM | 3678 | CB | VAL | 479 | 80.105 | 2.829 | -0.563 | 1.00 | 36.57 |
| ATOM | 3679 | CG1 | VAL | 479 | 79.647 | 3.105 | -1.994 | 1.00 | 31.59 |
| ATOM | 3680 | CG2 | VAL | 479 | 81.608 | 2.567 | -0.561 | 1.00 | 36.11 |
| ATOM | 3681 | C | VAL | 479 | 78.267 | 4.277 | 0.375 | 1.00 | 39.24 |
| ATOM | 3682 | O | VAL | 479 | 77.484 | 3.358 | 0.619 | 1.00 | 39.16 |
| ATOM | 3683 | N | LEU | 480 | 77.894 | 5.528 | 0.142 | 1.00 | 41.32 |
| ATOM | 3685 | CA | LEU | 480 | 76.505 | 5.960 | 0.123 | 1.00 | 41.60 |
| ATOM | 3686 | CB | LEU | 480 | 76.446 | 7.480 | -0.008 | 1.00 | 41.31 |
| ATOM | 3687 | CG | LEU | 480 | 77.129 | 8.257 | 1.118 | 1.00 | 39.82 |
| ATOM | 3688 | CD1 | LEU | 480 | 76.985 | 9.737 | 0.856 | 1.00 | 37.96 |
| ATOM | 3689 | CD2 | LEU | 480 | 76.512 | 7.887 | 2.458 | 1.00 | 37.70 |
| ATOM | 3690 | C | LEU | 480 | 75.733 | 5.312 | -1.015 | 1.00 | 41.85 |
| ATOM | 3691 | O | LEU | 480 | 76.235 | 5.224 | -2.131 | 1.00 | 45.02 |
| ATOM | 3692 | N | GLY | 481 | 74.501 | 4.897 | -0.727 | 1.00 | 40.86 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3694 | CA | GLY | 481 | 73.673 | 4.247 | -1.727 | 1.00 | 40.21 |
| ATOM | 3695 | C | GLY | 481 | 72.270 | 4.806 | -1.873 | 1.00 | 39.78 |
| ATOM | 3696 | O | GLY | 481 | 72.058 | 6.015 | -1.810 | 1.00 | 41.68 |
| ATOM | 3697 | N | LYS | 482 | 71.306 | 3.914 | -2.063 | 1.00 | 39.98 |
| ATOM | 3699 | CA | LYS | 482 | 69.910 | 4.297 | -2.249 | 1.00 | 42.13 |
| ATOM | 3700 | CB | LYS | 482 | 69.061 | 3.056 | -2.566 | 1.00 | 42.73 |
| ATOM | 3701 | C | LYS | 482 | 69.284 | 5.050 | -1.084 | 1.00 | 43.13 |
| ATOM | 3702 | O | LYS | 482 | 69.373 | 4.625 | 0.060 | 1.00 | 44.49 |
| ATOM | 3703 | N | PRO | 483 | 68.676 | 6.204 | -1.358 | 1.00 | 43.22 |
| ATOM | 3704 | CD | PRO | 483 | 68.708 | 6.969 | -2.613 | 1.00 | 44.40 |
| ATOM | 3705 | CA | PRO | 483 | 68.044 | 6.973 | -0.290 | 1.00 | 45.44 |
| ATOM | 3706 | CB | PRO | 483 | 67.701 | 8.295 | -0.980 | 1.00 | 45.01 |
| ATOM | 3707 | CG | PRO | 483 | 67.573 | 7.923 | -2.414 | 1.00 | 43.95 |
| ATOM | 3708 | C | PRO | 483 | 66.801 | 6.261 | 0.232 | 1.00 | 47.67 |
| ATOM | 3709 | O | PRO | 483 | 66.012 | 5.725 | -0.547 | 1.00 | 46.76 |
| ATOM | 3710 | N | LEU | 484 | 66.650 | 6.242 | 1.552 | 1.00 | 49.68 |
| ATOM | 3712 | CA | LEU | 484 | 65.514 | 5.598 | 2.196 | 1.00 | 54.51 |
| ATOM | 3713 | CB | LEU | 484 | 65.935 | 5.026 | 3.555 | 1.00 | 52.70 |
| ATOM | 3714 | CG | LEU | 484 | 67.132 | 4.066 | 3.530 | 1.00 | 51.83 |
| ATOM | 3715 | CD1 | LEU | 484 | 67.620 | 3.766 | 4.933 | 1.00 | 50.19 |
| ATOM | 3716 | CD2 | LEU | 484 | 66.755 | 2.788 | 2.825 | 1.00 | 52.22 |
| ATOM | 3717 | C | LEU | 484 | 64.317 | 6.554 | 2.357 | 1.00 | 58.82 |
| ATOM | 3718 | O | LEU | 484 | 63.158 | 6.138 | 2.244 | 1.00 | 60.07 |
| ATOM | 3719 | N | GLY | 485 | 64.599 | 7.831 | 2.609 | 1.00 | 61.91 |
| ATOM | 3721 | CA | GLY | 485 | 63.538 | 8.810 | 2.778 | 1.00 | 65.89 |
| ATOM | 3722 | C | GLY | 485 | 64.057 | 10.167 | 3.227 | 1.00 | 69.46 |
| ATOM | 3723 | O | GLY | 485 | 65.230 | 10.301 | 3.597 | 1.00 | 70.65 |
| ATOM | 3724 | N | GLU | 486 | 63.178 | 11.165 | 3.241 | 1.00 | 70.72 |
| ATOM | 3726 | CA | GLU | 486 | 63.563 | 12.521 | 3.624 | 1.00 | 71.32 |
| ATOM | 3727 | CB | GLU | 486 | 64.015 | 13.298 | 2.389 | 1.00 | 73.69 |
| ATOM | 3728 | C | GLU | 486 | 62.435 | 13.269 | 4.312 | 1.00 | 70.93 |
| ATOM | 3729 | O | GLU | 486 | 61.281 | 12.846 | 4.275 | 1.00 | 71.58 |
| ATOM | 3730 | N | GLY | 487 | 62.781 | 14.404 | 4.909 | 1.00 | 70.10 |
| ATOM | 3732 | CA | GLY | 487 | 61.798 | 15.211 | 5.603 | 1.00 | 68.11 |
| ATOM | 3733 | C | GLY | 487 | 62.218 | 16.669 | 5.598 | 1.00 | 67.97 |
| ATOM | 3734 | O | GLY | 487 | 62.938 | 17.109 | 4.696 | 1.00 | 67.68 |
| ATOM | 3735 | N | ALA | 488 | 61.780 | 17.409 | 6.615 | 1.00 | 67.26 |
| ATOM | 3737 | CA | ALA | 488 | 62.106 | 18.826 | 6.737 | 1.00 | 66.90 |
| ATOM | 3738 | CB | ALA | 488 | 61.362 | 19.428 | 7.909 | 1.00 | 68.72 |
| ATOM | 3739 | C | ALA | 488 | 63.607 | 19.004 | 6.921 | 1.00 | 67.08 |
| ATOM | 3740 | O | ALA | 488 | 64.124 | 18.867 | 8.037 | 1.00 | 65.97 |
| ATOM | 3741 | N | PHE | 489 | 64.297 | 19.248 | 5.806 | 1.00 | 66.76 |
| ATOM | 3743 | CA | PHE | 489 | 65.754 | 19.439 | 5.773 | 1.00 | 65.91 |
| ATOM | 3744 | CB | PHE | 489 | 66.134 | 20.794 | 6.379 | 1.00 | 66.45 |
| ATOM | 3745 | C | PHE | 489 | 66.563 | 18.288 | 6.414 | 1.00 | 63.92 |
| ATOM | 3746 | O | PHE | 489 | 67.622 | 18.503 | 7.031 | 1.00 | 63.16 |
| ATOM | 3747 | N | GLY | 490 | 66.067 | 17.069 | 6.209 | 1.00 | 59.03 |
| ATOM | 3749 | CA | GLY | 490 | 66.710 | 15.878 | 6.720 | 1.00 | 51.12 |
| ATOM | 3750 | C | GLY | 490 | 66.619 | 14.823 | 5.638 | 1.00 | 48.59 |
| ATOM | 3751 | O | GLY | 490 | 65.608 | 14.736 | 4.938 | 1.00 | 45.25 |
| ATOM | 3752 | N | GLN | 491 | 67.659 | 14.003 | 5.525 | 1.00 | 48.77 |
| ATOM | 3754 | CA | GLN | 491 | 67.732 | 12.951 | 4.519 | 1.00 | 47.40 |
| ATOM | 3755 | CB | GLN | 491 | 68.529 | 13.474 | 3.319 | 1.00 | 49.92 |
| ATOM | 3756 | CG | GLN | 491 | 68.653 | 12.514 | 2.155 | 1.00 | 56.31 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3757 | CD | GLN | 491 | 69.604 | 13.020 | 1.088 | 1.00 | 58.79 |
| ATOM | 3758 | OE1 | GLN | 491 | 70.043 | 14.171 | 1.130 | 1.00 | 59.63 |
| ATOM | 3759 | NE2 | GLN | 491 | 69.929 | 12.161 | 0.122 | 1.00 | 59.05 |
| ATOM | 3762 | C | GLN | 491 | 68.407 | 11.693 | 5.086 | 1.00 | 44.46 |
| ATOM | 3763 | O | GLN | 491 | 69.396 | 11.782 | 5.806 | 1.00 | 44.15 |
| ATOM | 3764 | N | VAL | 492 | 67.867 | 10.527 | 4.752 | 1.00 | 42.55 |
| ATOM | 3766 | CA | VAL | 492 | 68.416 | 9.247 | 5.205 | 1.00 | 39.22 |
| ATOM | 3767 | CB | VAL | 492 | 67.375 | 8.458 | 6.042 | 1.00 | 39.40 |
| ATOM | 3768 | CG1 | VAL | 492 | 67.947 | 7.127 | 6.524 | 1.00 | 40.17 |
| ATOM | 3769 | CG2 | VAL | 492 | 66.922 | 9.267 | 7.210 | 1.00 | 36.12 |
| ATOM | 3770 | C | VAL | 492 | 68.746 | 8.396 | 3.975 | 1.00 | 37.57 |
| ATOM | 3771 | O | VAL | 492 | 67.888 | 8.178 | 3.115 | 1.00 | 35.70 |
| ATOM | 3772 | N | VAL | 493 | 69.990 | 7.961 | 3.845 | 1.00 | 36.27 |
| ATOM | 3774 | CA | VAL | 493 | 70.333 | 7.127 | 2.711 | 1.00 | 37.61 |
| ATOM | 3775 | CB | VAL | 493 | 71.237 | 7.863 | 1.643 | 1.00 | 37.45 |
| ATOM | 3776 | CG1 | VAL | 493 | 70.836 | 9.319 | 1.524 | 1.00 | 38.29 |
| ATOM | 3777 | CG2 | VAL | 493 | 72.717 | 7.713 | 1.943 | 1.00 | 36.53 |
| ATOM | 3778 | C | VAL | 493 | 70.952 | 5.806 | 3.156 | 1.00 | 37.54 |
| ATOM | 3779 | O | VAL | 493 | 71.542 | 5.711 | 4.233 | 1.00 | 37.32 |
| ATOM | 3780 | N | LEU | 494 | 70.691 | 4.763 | 2.380 | 1.00 | 37.67 |
| ATOM | 3782 | CA | LEU | 494 | 71.236 | 3.450 | 2.656 | 1.00 | 38.41 |
| ATOM | 3783 | CB | LEU | 494 | 70.482 | 2.387 | 1.851 | 1.00 | 39.16 |
| ATOM | 3784 | CG | LEU | 494 | 70.834 | 0.908 | 2.021 | 1.00 | 36.43 |
| ATOM | 3785 | CD1 | LEU | 494 | 70.809 | 0.508 | 3.479 | 1.00 | 34.69 |
| ATOM | 3786 | CD2 | LEU | 494 | 69.840 | 0.086 | 1.229 | 1.00 | 37.48 |
| ATOM | 3787 | C | LEU | 494 | 72.683 | 3.541 | 2.202 | 1.00 | 39.30 |
| ATOM | 3788 | O | LEU | 494 | 72.976 | 4.201 | 1.207 | 1.00 | 39.21 |
| ATOM | 3789 | N | ALA | 495 | 73.584 | 2.922 | 2.954 | 1.00 | 40.08 |
| ATOM | 3791 | CA | ALA | 495 | 74.996 | 2.954 | 2.619 | 1.00 | 41.70 |
| ATOM | 3792 | CB | ALA | 495 | 75.654 | 4.162 | 3.283 | 1.00 | 41.63 |
| ATOM | 3793 | C | ALA | 495 | 75.670 | 1.669 | 3.080 | 1.00 | 43.92 |
| ATOM | 3794 | O | ALA | 495 | 75.033 | 0.818 | 3.711 | 1.00 | 45.20 |
| ATOM | 3795 | N | GLU | 496 | 76.946 | 1.515 | 2.731 | 1.00 | 44.21 |
| ATOM | 3797 | CA | GLU | 496 | 77.712 | 0.347 | 3.137 | 1.00 | 43.44 |
| ATOM | 3798 | CB | GLU | 496 | 78.046 | -0.538 | 1.943 | 1.00 | 45.87 |
| ATOM | 3799 | CG | GLU | 496 | 76.816 | -1.142 | 1.301 | 1.00 | 53.11 |
| ATOM | 3800 | CD | GLU | 496 | 77.145 | -2.262 | 0.339 | 1.00 | 56.68 |
| ATOM | 3801 | OE1 | GLU | 496 | 76.473 | -3.316 | 0.410 | 1.00 | 61.87 |
| ATOM | 3802 | OE2 | GLU | 496 | 78.068 | -2.091 | -0.482 | 1.00 | 58.18 |
| ATOM | 3803 | C | GLU | 496 | 78.973 | 0.773 | 3.860 | 1.00 | 40.97 |
| ATOM | 3804 | O | GLU | 496 | 79.835 | 1.437 | 3.302 | 1.00 | 40.91 |
| ATOM | 3805 | N | ALA | 497 | 79.036 | 0.439 | 5.136 | 1.00 | 42.07 |
| ATOM | 3807 | CA | ALA | 497 | 80.173 | 0.786 | 5.959 | 1.00 | 43.69 |
| ATOM | 3808 | CB | ALA | 497 | 79.709 | 1.104 | 7.366 | 1.00 | 40.90 |
| ATOM | 3809 | C | ALA | 497 | 81.160 | -0.372 | 5.962 | 1.00 | 46.16 |
| ATOM | 3810 | O | ALA | 497 | 80.764 | -1.525 | 5.814 | 1.00 | 46.90 |
| ATOM | 3811 | N | ILE | 498 | 82.446 | -0.059 | 6.090 | 1.00 | 48.78 |
| ATOM | 3813 | CA | ILE | 498 | 83.494 | -1.068 | 6.114 | 1.00 | 49.59 |
| ATOM | 3814 | CB | ILE | 498 | 84.395 | -0.993 | 4.858 | 1.00 | 49.46 |
| ATOM | 3815 | CG2 | ILE | 498 | 85.524 | -2.006 | 4.954 | 1.00 | 51.16 |
| ATOM | 3816 | CG1 | ILE | 498 | 83.577 | -1.244 | 3.591 | 1.00 | 48.96 |
| ATOM | 3817 | CD1 | ILE | 498 | 82.924 | 0.009 | 2.998 | 1.00 | 52.50 |
| ATOM | 3818 | C | ILE | 498 | 84.352 | -0.877 | 7.355 | 1.00 | 51.33 |
| ATOM | 3819 | O | ILE | 498 | 84.818 | 0.230 | 7.641 | 1.00 | 50.42 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3820 | N | GLY | 499 | 84.506 | -1.952 | 8.119 | 1.00 | 53.87 |
| ATOM | 3822 | CA | GLY | 499 | 85.314 | -1.909 | 9.324 | 1.00 | 58.16 |
| ATOM | 3823 | C | GLY | 499 | 84.759 | -1.094 | 10.483 | 1.00 | 62.44 |
| ATOM | 3824 | O | GLY | 499 | 85.510 | -0.400 | 11.175 | 1.00 | 65.17 |
| ATOM | 3825 | N | LEU | 500 | 83.454 | -1.187 | 10.720 | 1.00 | 62.92 |
| ATOM | 3827 | CA | LEU | 500 | 82.839 | -0.453 | 11.822 | 1.00 | 61.93 |
| ATOM | 3828 | CB | LEU | 500 | 81.339 | -0.752 | 11.888 | 1.00 | 58.77 |
| ATOM | 3829 | CG | LEU | 500 | 80.501 | -0.207 | 10.736 | 1.00 | 56.68 |
| ATOM | 3830 | CD1 | LEU | 500 | 79.047 | -0.547 | 10.964 | 1.00 | 55.05 |
| ATOM | 3831 | CD2 | LEU | 500 | 80.682 | 1.298 | 10.635 | 1.00 | 56.30 |
| ATOM | 3832 | C | LEU | 500 | 83.501 | -0.820 | 13.149 | 1.00 | 63.28 |
| ATOM | 3833 | O | LEU | 500 | 83.623 | -2.002 | 13.487 | 1.00 | 64.91 |
| ATOM | 3834 | N | PRO | 505 | 87.387 | -6.451 | 10.091 | 1.00 | 82.92 |
| ATOM | 3835 | CD | PRO | 505 | 88.522 | -6.966 | 10.874 | 1.00 | 83.74 |
| ATOM | 3836 | CA | PRO | 505 | 87.618 | -5.052 | 9.705 | 1.00 | 80.73 |
| ATOM | 3837 | CB | PRO | 505 | 89.027 | -4.770 | 10.247 | 1.00 | 81.95 |
| ATOM | 3838 | CG | PRO | 505 | 89.655 | -6.133 | 10.342 | 1.00 | 83.54 |
| ATOM | 3839 | C | PRO | 505 | 87.514 | -4.794 | 8.205 | 1.00 | 77.60 |
| ATOM | 3840 | O | PRO | 505 | 87.445 | -3.651 | 7.761 | 1.00 | 77.24 |
| ATOM | 3841 | N | ASN | 506 | 87.488 | -5.863 | 7.424 | 1.00 | 75.24 |
| ATOM | 3843 | CA | ASN | 506 | 87.380 | -5.727 | 5.981 | 1.00 | 72.92 |
| ATOM | 3844 | CB | ASN | 506 | 88.435 | -6.589 | 5.283 | 1.00 | 73.87 |
| ATOM | 3845 | C | ASN | 506 | 85.978 | -6.122 | 5.529 | 1.00 | 70.43 |
| ATOM | 3846 | O | ASN | 506 | 85.719 | -6.281 | 4.340 | 1.00 | 70.01 |
| ATOM | 3847 | N | ARG | 507 | 85.075 | -6.273 | 6.491 | 1.00 | 68.31 |
| ATOM | 3849 | CA | ARG | 507 | 83.697 | -6.647 | 6.200 | 1.00 | 65.59 |
| ATOM | 3850 | CB | ARG | 507 | 83.112 | -7.429 | 7.378 | 1.00 | 66.34 |
| ATOM | 3851 | C | ARG | 507 | 82.846 | -5.413 | 5.941 | 1.00 | 62.97 |
| ATOM | 3852 | O | ARG | 507 | 83.191 | -4.313 | 6.375 | 1.00 | 63.16 |
| ATOM | 3853 | N | VAL | 508 | 81.740 | -5.599 | 5.231 | 1.00 | 60.02 |
| ATOM | 3855 | CA | VAL | 508 | 80.840 | -4.495 | 4.947 | 1.00 | 58.59 |
| ATOM | 3856 | CB | VAL | 508 | 80.532 | -4.357 | 3.439 | 1.00 | 58.40 |
| ATOM | 3857 | CG1 | VAL | 508 | 81.813 | -4.196 | 2.658 | 1.00 | 61.14 |
| ATOM | 3858 | CG2 | VAL | 508 | 79.751 | -5.553 | 2.938 | 1.00 | 61.01 |
| ATOM | 3859 | C | VAL | 508 | 79.537 | -4.682 | 5.707 | 1.00 | 57.24 |
| ATOM | 3860 | O | VAL | 508 | 79.031 | -5.803 | 5.836 | 1.00 | 58.42 |
| ATOM | 3861 | N | THR | 509 | 79.020 | -3.579 | 6.237 | 1.00 | 54.22 |
| ATOM | 3863 | CA | THR | 509 | 77.769 | -3.572 | 6.973 | 1.00 | 48.99 |
| ATOM | 3864 | CB | THR | 509 | 77.971 | -3.100 | 8.428 | 1.00 | 49.59 |
| ATOM | 3865 | OG1 | THR | 509 | 78.932 | -3.935 | 9.082 | 1.00 | 51.71 |
| ATOM | 3867 | CG2 | THR | 509 | 76.665 | -3.166 | 9.198 | 1.00 | 50.69 |
| ATOM | 3868 | C | THR | 509 | 76.837 | -2.606 | 6.253 | 1.00 | 46.51 |
| ATOM | 3869 | O | THR | 509 | 77.231 | -1.503 | 5.886 | 1.00 | 44.91 |
| ATOM | 3870 | N | LYS | 510 | 75.628 | -3.059 | 5.966 | 1.00 | 45.65 |
| ATOM | 3872 | CA | LYS | 510 | 74.658 | -2.208 | 5.314 | 1.00 | 43.61 |
| ATOM | 3873 | CB | LYS | 510 | 73.598 | -3.058 | 4.632 | 1.00 | 45.46 |
| ATOM | 3874 | CG | LYS | 510 | 72.845 | -2.306 | 3.568 | 1.00 | 54.00 |
| ATOM | 3875 | CD | LYS | 510 | 73.022 | -2.912 | 2.183 | 1.00 | 58.74 |
| ATOM | 3876 | CE | LYS | 510 | 72.194 | -4.184 | 2.007 | 1.00 | 59.63 |
| ATOM | 3877 | NZ | LYS | 510 | 72.711 | -5.323 | 2.815 | 1.00 | 61.62 |
| ATOM | 3881 | C | LYS | 510 | 74.065 | -1.359 | 6.450 | 1.00 | 42.05 |
| ATOM | 3882 | O | LYS | 510 | 73.566 | -1.898 | 7.439 | 1.00 | 41.29 |
| ATOM | 3883 | N | VAL | 511 | 74.185 | -0.038 | 6.333 | 1.00 | 40.14 |
| ATOM | 3885 | CA | VAL | 511 | 73.719 | 0.894 | 7.359 | 1.00 | 35.38 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3886 | CB | VAL | 511 | 74.932 | 1.554 | 8.074 | 1.00 | 33.16 |
| ATOM | 3887 | CG1 | VAL | 511 | 75.761 | 0.501 | 8.795 | 1.00 | 29.24 |
| ATOM | 3888 | CG2 | VAL | 511 | 75.804 | 2.295 | 7.054 | 1.00 | 30.37 |
| ATOM | 3889 | C | VAL | 511 | 72.856 | 2.005 | 6.776 | 1.00 | 33.90 |
| ATOM | 3890 | O | VAL | 511 | 72.722 | 2.110 | 5.558 | 1.00 | 32.53 |
| ATOM | 3891 | N | ALA | 512 | 72.261 | 2.813 | 7.655 | 1.00 | 31.97 |
| ATOM | 3893 | CA | ALA | 512 | 71.434 | 3.956 | 7.248 | 1.00 | 31.10 |
| ATOM | 3894 | CB | ALA | 512 | 70.088 | 3.945 | 7.952 | 1.00 | 27.38 |
| ATOM | 3895 | C | ALA | 512 | 72.225 | 5.186 | 7.660 | 1.00 | 30.49 |
| ATOM | 3896 | O | ALA | 512 | 72.775 | 5.235 | 8.766 | 1.00 | 30.10 |
| ATOM | 3897 | N | VAL | 513 | 72.312 | 6.162 | 6.765 | 1.00 | 30.50 |
| ATOM | 3899 | CA | VAL | 513 | 73.064 | 7.382 | 7.041 | 1.00 | 29.68 |
| ATOM | 3900 | CB | VAL | 513 | 74.204 | 7.593 | 6.015 | 1.00 | 28.89 |
| ATOM | 3901 | CG1 | VAL | 513 | 74.966 | 8.856 | 6.334 | 1.00 | 26.30 |
| ATOM | 3902 | CG2 | VAL | 513 | 75.134 | 6.389 | 5.987 | 1.00 | 26.66 |
| ATOM | 3903 | C | VAL | 513 | 72.171 | 8.607 | 7.012 | 1.00 | 28.50 |
| ATOM | 3904 | O | VAL | 513 | 71.536 | 8.893 | 5.994 | 1.00 | 26.27 |
| ATOM | 3905 | N | LYS | 514 | 72.091 | 9.282 | 8.154 | 1.00 | 29.18 |
| ATOM | 3907 | CA | LYS | 514 | 71.307 | 10.508 | 8.295 | 1.00 | 31.52 |
| ATOM | 3908 | CB | LYS | 514 | 70.797 | 10.659 | 9.728 | 1.00 | 33.52 |
| ATOM | 3909 | CG | LYS | 514 | 69.890 | 9.540 | 10.198 | 1.00 | 35.67 |
| ATOM | 3910 | CD | LYS | 514 | 69.439 | 9.831 | 11.618 | 1.00 | 44.89 |
| ATOM | 3911 | CE | LYS | 514 | 68.313 | 8.909 | 12.060 | 1.00 | 51.12 |
| ATOM | 3912 | NZ | LYS | 514 | 67.029 | 9.137 | 11.307 | 1.00 | 57.11 |
| ATOM | 3916 | C | LYS | 514 | 72.233 | 11.681 | 7.956 | 1.00 | 30.75 |
| ATOM | 3917 | O | LYS | 514 | 73.390 | 11.698 | 8.379 | 1.00 | 30.08 |
| ATOM | 3918 | N | MET | 515 | 71.724 | 12.651 | 7.201 | 1.00 | 29.45 |
| ATOM | 3920 | CA | MET | 515 | 72.511 | 13.814 | 6.786 | 1.00 | 28.74 |
| ATOM | 3921 | CB | MET | 515 | 73.342 | 13.466 | 5.552 | 1.00 | 27.72 |
| ATOM | 3922 | CG | MET | 515 | 72.487 | 13.034 | 4.378 | 1.00 | 31.56 |
| ATOM | 3923 | SD | MET | 515 | 73.442 | 12.549 | 2.945 | 1.00 | 34.98 |
| ATOM | 3924 | CE | MET | 515 | 73.730 | 10.878 | 3.330 | 1.00 | 31.23 |
| ATOM | 3925 | C | MET | 515 | 71.585 | 14.966 | 6.444 | 1.00 | 27.75 |
| ATOM | 3926 | O | MET | 515 | 70.369 | 14.794 | 6.359 | 1.00 | 29.07 |
| ATOM | 3927 | N | LEU | 516 | 72.152 | 16.145 | 6.247 | 1.00 | 28.33 |
| ATOM | 3929 | CA | LEU | 516 | 71.348 | 17.313 | 5.912 | 1.00 | 31.16 |
| ATOM | 3930 | CB | LEU | 516 | 72.052 | 18.605 | 6.339 | 1.00 | 28.70 |
| ATOM | 3931 | CG | LEU | 516 | 72.312 | 18.866 | 7.826 | 1.00 | 28.33 |
| ATOM | 3932 | CD1 | LEU | 516 | 73.098 | 20.156 | 7.949 | 1.00 | 28.45 |
| ATOM | 3933 | CD2 | LEU | 516 | 71.020 | 18.959 | 8.604 | 1.00 | 21.64 |
| ATOM | 3934 | C | LEU | 516 | 71.069 | 17.378 | 4.421 | 1.00 | 33.22 |
| ATOM | 3935 | O | LEU | 516 | 71.762 | 16.760 | 3.619 | 1.00 | 35.00 |
| ATOM | 3936 | N | LYS | 517 | 70.022 | 18.100 | 4.061 | 1.00 | 34.69 |
| ATOM | 3938 | CA | LYS | 517 | 69.696 | 18.286 | 2.665 | 1.00 | 34.20 |
| ATOM | 3939 | CB | LYS | 517 | 68.194 | 18.475 | 2.496 | 1.00 | 37.45 |
| ATOM | 3940 | CG | LYS | 517 | 67.403 | 17.264 | 2.950 | 1.00 | 43.71 |
| ATOM | 3941 | CD | LYS | 517 | 66.157 | 17.072 | 2.126 | 1.00 | 51.25 |
| ATOM | 3942 | CE | LYS | 517 | 65.123 | 18.135 | 2.419 | 1.00 | 58.56 |
| ATOM | 3943 | NZ | LYS | 517 | 64.010 | 18.049 | 1.438 | 1.00 | 63.12 |
| ATOM | 3947 | C | LYS | 517 | 70.482 | 19.533 | 2.259 | 1.00 | 33.81 |
| ATOM | 3948 | O | LYS | 517 | 70.991 | 20.244 | 3.130 | 1.00 | 33.17 |
| ATOM | 3949 | N | SER | 518 | 70.603 | 19.788 | 0.959 | 1.00 | 33.42 |
| ATOM | 3951 | CA | SER | 518 | 71.369 | 20.938 | 0.472 | 1.00 | 33.33 |
| ATOM | 3952 | CB | SER | 518 | 71.550 | 20.842 | -1.042 | 1.00 | 33.23 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3953 | OG | SER | 518 | 70.306 | 20.624 | -1.678 | 1.00 | 38.84 |
| ATOM | 3955 | C | SER | 518 | 70.794 | 22.298 | 0.846 | 1.00 | 33.23 |
| ATOM | 3956 | O | SER | 518 | 71.509 | 23.305 | 0.865 | 1.00 | 34.14 |
| ATOM | 3957 | N | ASP | 519 | 69.510 | 22.313 | 1.178 | 1.00 | 32.77 |
| ATOM | 3959 | CA | ASP | 519 | 68.825 | 23.541 | 1.570 | 1.00 | 33.26 |
| ATOM | 3960 | CB | ASP | 519 | 67.401 | 23.563 | 0.995 | 1.00 | 35.10 |
| ATOM | 3961 | CG | ASP | 519 | 66.484 | 22.503 | 1.617 | 1.00 | 38.98 |
| ATOM | 3962 | OD1 | ASP | 519 | 66.958 | 21.430 | 2.042 | 1.00 | 37.30 |
| ATOM | 3963 | OD2 | ASP | 519 | 65.261 | 22.754 | 1.674 | 1.00 | 43.65 |
| ATOM | 3964 | C | ASP | 519 | 68.793 | 23.747 | 3.091 | 1.00 | 33.05 |
| ATOM | 3965 | O | ASP | 519 | 68.114 | 24.648 | 3.580 | 1.00 | 35.19 |
| ATOM | 3966 | N | ALA | 520 | 69.538 | 22.931 | 3.833 | 1.00 | 31.38 |
| ATOM | 3968 | CA | ALA | 520 | 69.570 | 23.032 | 5.293 | 1.00 | 29.47 |
| ATOM | 3969 | CB | ALA | 520 | 70.264 | 21.830 | 5.870 | 1.00 | 29.74 |
| ATOM | 3970 | C | ALA | 520 | 70.229 | 24.301 | 5.812 | 1.00 | 29.83 |
| ATOM | 3971 | O | ALA | 520 | 71.004 | 24.952 | 5.106 | 1.00 | 30.23 |
| ATOM | 3972 | N | THR | 521 | 69.938 | 24.616 | 7.071 | 1.00 | 31.57 |
| ATOM | 3974 | CA | THR | 521 | 70.487 | 25.793 | 7.742 | 1.00 | 34.56 |
| ATOM | 3975 | CB | THR | 521 | 69.361 | 26.736 | 8.302 | 1.00 | 38.37 |
| ATOM | 3976 | OG1 | THR | 521 | 68.670 | 26.082 | 9.376 | 1.00 | 41.75 |
| ATOM | 3978 | CG2 | THR | 521 | 68.357 | 27.117 | 7.209 | 1.00 | 38.30 |
| ATOM | 3979 | C | THR | 521 | 71.353 | 25.363 | 8.916 | 1.00 | 33.22 |
| ATOM | 3980 | O | THR | 521 | 71.320 | 24.207 | 9.327 | 1.00 | 32.31 |
| ATOM | 3981 | N | GLU | 522 | 72.092 | 26.310 | 9.479 | 1.00 | 34.43 |
| ATOM | 3983 | CA | GLU | 522 | 72.951 | 26.042 | 10.619 | 1.00 | 39.53 |
| ATOM | 3984 | CB | GLU | 522 | 73.634 | 27.340 | 11.068 | 1.00 | 46.35 |
| ATOM | 3985 | CG | GLU | 522 | 74.398 | 27.271 | 12.402 | 1.00 | 58.03 |
| ATOM | 3986 | CD | GLU | 522 | 75.772 | 26.603 | 12.301 | 1.00 | 63.14 |
| ATOM | 3987 | OE1 | GLU | 522 | 76.800 | 27.321 | 12.404 | 1.00 | 61.75 |
| ATOM | 3988 | OE2 | GLU | 522 | 75.824 | 25.359 | 12.158 | 1.00 | 66.35 |
| ATOM | 3989 | C | GLU | 522 | 72.130 | 25.428 | 11.765 | 1.00 | 38.40 |
| ATOM | 3990 | O | GLU | 522 | 72.642 | 24.622 | 12.543 | 1.00 | 37.92 |
| ATOM | 3991 | N | LYS | 523 | 70.853 | 25.792 | 11.849 | 1.00 | 36.43 |
| ATOM | 3993 | CA | LYS | 523 | 69.995 | 25.261 | 12.893 | 1.00 | 36.83 |
| ATOM | 3994 | CB | LYS | 523 | 68.703 | 26.065 | 13.008 | 1.00 | 40.88 |
| ATOM | 3995 | CG | LYS | 523 | 67.793 | 25.636 | 14.152 | 1.00 | 44.55 |
| ATOM | 3996 | CD | LYS | 523 | 66.584 | 24.898 | 13.607 | 1.00 | 52.68 |
| ATOM | 3997 | CE | LYS | 523 | 65.629 | 24.483 | 14.708 | 1.00 | 56.04 |
| ATOM | 3998 | NZ | LYS | 523 | 64.537 | 23.646 | 14.123 | 1.00 | 58.13 |
| ATOM | 4002 | C | LYS | 523 | 69.689 | 23.804 | 12.601 | 1.00 | 35.27 |
| ATOM | 4003 | O | LYS | 523 | 69.645 | 22.985 | 13.513 | 1.00 | 36.58 |
| ATOM | 4004 | N | ASP | 524 | 69.496 | 23.473 | 11.326 | 1.00 | 32.27 |
| ATOM | 4006 | CA | ASP | 524 | 69.235 | 22.089 | 10.963 | 1.00 | 27.18 |
| ATOM | 4007 | CB | ASP | 524 | 68.952 | 21.953 | 9.480 | 1.00 | 26.32 |
| ATOM | 4008 | CG | ASP | 524 | 67.635 | 22.555 | 9.089 | 1.00 | 25.22 |
| ATOM | 4009 | OD1 | ASP | 524 | 66.662 | 22.394 | 9.848 | 1.00 | 31.78 |
| ATOM | 4010 | OD2 | ASP | 524 | 67.568 | 23.190 | 8.028 | 1.00 | 24.00 |
| ATOM | 4011 | C | ASP | 524 | 70.445 | 21.268 | 11.342 | 1.00 | 26.83 |
| ATOM | 4012 | O | ASP | 524 | 70.312 | 20.165 | 11.851 | 1.00 | 28.65 |
| ATOM | 4013 | N | LEU | 525 | 71.633 | 21.827 | 11.129 | 1.00 | 28.69 |
| ATOM | 4015 | CA | LEU | 525 | 72.872 | 21.148 | 11.473 | 1.00 | 26.96 |
| ATOM | 4016 | CB | LEU | 525 | 74.077 | 21.981 | 11.049 | 1.00 | 22.80 |
| ATOM | 4017 | CG | LEU | 525 | 75.445 | 21.355 | 11.341 | 1.00 | 22.32 |
| ATOM | 4018 | CD1 | LEU | 525 | 75.522 | 19.883 | 10.858 | 1.00 | 18.89 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4019 | CD2 | LEU | 525 | 76.504 | 22.212 | 10.704 | 1.00 | 17.44 |
| ATOM | 4020 | C | LEU | 525 | 72.886 | 20.926 | 12.980 | 1.00 | 28.00 |
| ATOM | 4021 | O | LEU | 525 | 73.160 | 19.816 | 13.462 | 1.00 | 28.82 |
| ATOM | 4022 | N | SER | 526 | 72.567 | 21.992 | 13.707 | 1.00 | 27.98 |
| ATOM | 4024 | CA | SER | 526 | 72.496 | 21.994 | 15.168 | 1.00 | 30.78 |
| ATOM | 4025 | CB | SER | 526 | 71.939 | 23.345 | 15.627 | 1.00 | 33.18 |
| ATOM | 4026 | OG | SER | 526 | 71.624 | 23.347 | 17.009 | 1.00 | 42.73 |
| ATOM | 4028 | C | SER | 526 | 71.599 | 20.865 | 15.704 | 1.00 | 30.56 |
| ATOM | 4029 | O | SER | 526 | 71.906 | 20.206 | 16.716 | 1.00 | 31.92 |
| ATOM | 4030 | N | ASP | 527 | 70.484 | 20.665 | 15.018 | 1.00 | 28.19 |
| ATOM | 4032 | CA | ASP | 527 | 69.516 | 19.651 | 15.366 | 1.00 | 27.41 |
| ATOM | 4033 | CB | ASP | 527 | 68.207 | 19.932 | 14.632 | 1.00 | 27.63 |
| ATOM | 4034 | CG | ASP | 527 | 67.492 | 21.172 | 15.149 | 1.00 | 27.37 |
| ATOM | 4035 | OD1 | ASP | 527 | 67.870 | 21.728 | 16.211 | 1.00 | 26.70 |
| ATOM | 4036 | OD2 | ASP | 527 | 66.525 | 21.579 | 14.487 | 1.00 | 33.80 |
| ATOM | 4037 | C | ASP | 527 | 70.007 | 18.241 | 15.063 | 1.00 | 27.36 |
| ATOM | 4038 | O | ASP | 527 | 69.722 | 17.309 | 15.816 | 1.00 | 30.13 |
| ATOM | 4039 | N | LEU | 528 | 70.716 | 18.077 | 13.952 | 1.00 | 25.76 |
| ATOM | 4041 | CA | LEU | 528 | 71.245 | 16.765 | 13.588 | 1.00 | 25.29 |
| ATOM | 4042 | CB | LEU | 528 | 71.777 | 16.771 | 12.143 | 1.00 | 23.65 |
| ATOM | 4043 | CG | LEU | 528 | 72.283 | 15.432 | 11.574 | 1.00 | 25.86 |
| ATOM | 4044 | CD1 | LEU | 528 | 71.234 | 14.341 | 11.770 | 1.00 | 23.35 |
| ATOM | 4045 | CD2 | LEU | 528 | 72.652 | 15.566 | 10.102 | 1.00 | 17.46 |
| ATOM | 4046 | C | LEU | 528 | 72.351 | 16.368 | 14.578 | 1.00 | 25.66 |
| ATOM | 4047 | C | LEU | 528 | 72.418 | 15.210 | 15.015 | 1.00 | 24.02 |
| ATOM | 4048 | N | ILE | 529 | 73.200 | 17.338 | 14.934 | 1.00 | 26.36 |
| ATOM | 4050 | CA | ILE | 529 | 74.304 | 17.130 | 15.886 | 1.00 | 26.17 |
| ATOM | 4051 | CB | ILE | 529 | 75.192 | 18.381 | 16.003 | 1.00 | 22.72 |
| ATOM | 4052 | CG2 | ILE | 529 | 76.250 | 18.180 | 17.057 | 1.00 | 21.32 |
| ATOM | 4053 | CG1 | ILE | 529 | 75.876 | 18.666 | 14.685 | 1.00 | 20.71 |
| ATOM | 4054 | CD1 | ILE | 529 | 76.621 | 19.965 | 14.675 | 1.00 | 25.60 |
| ATOM | 4055 | C | ILE | 529 | 73.756 | 16.835 | 17.283 | 1.00 | 29.87 |
| ATOM | 4056 | O | ILE | 529 | 74.253 | 15.948 | 17.977 | 1.00 | 32.20 |
| ATOM | 4057 | N | SER | 530 | 72.741 | 17.591 | 17.693 | 1.00 | 28.63 |
| ATOM | 4059 | CA | SER | 530 | 72.143 | 17.381 | 18.991 | 1.00 | 32.21 |
| ATOM | 4060 | CB | SER | 530 | 71.031 | 18.399 | 19.231 | 1.00 | 37.45 |
| ATOM | 4061 | OG | SER | 530 | 70.065 | 18.342 | 18.195 | 1.00 | 49.52 |
| ATOM | 4063 | C | SER | 530 | 71.598 | 15.956 | 19.075 | 1.00 | 30.96 |
| ATOM | 4064 | O | SER | 530 | 71.728 | 15.301 | 20.105 | 1.00 | 33.05 |
| ATOM | 4065 | N | GLU | 531 | 70.996 | 15.476 | 17.996 | 1.00 | 29.13 |
| ATOM | 4067 | CA | GLU | 531 | 70.468 | 14.117 | 17.987 | 1.00 | 29.84 |
| ATOM | 4068 | CB | GLU | 531 | 69.672 | 13.847 | 16.709 | 1.00 | 30.29 |
| ATOM | 4069 | CG | GLU | 531 | 69.093 | 12.445 | 16.666 | 1.00 | 27.39 |
| ATOM | 4070 | CD | GLU | 531 | 68.521 | 12.074 | 15.331 | 1.00 | 31.34 |
| ATOM | 4071 | OE1 | GLU | 531 | 67.929 | 10.981 | 15.228 | 1.00 | 35.90 |
| ATOM | 4072 | OE2 | GLU | 531 | 68.660 | 12.860 | 14.376 | 1.00 | 38.37 |
| ATOM | 4073 | C | GLU | 531 | 71.600 | 13.081 | 18.109 | 1.00 | 28.48 |
| ATOM | 4074 | O | GLU | 531 | 71.468 | 12.094 | 18.822 | 1.00 | 28.17 |
| ATOM | 4075 | N | MET | 532 | 72.682 | 13.281 | 17.364 | 1.00 | 28.12 |
| ATOM | 4077 | CA | MET | 532 | 73.832 | 12.376 | 17.409 | 1.00 | 27.64 |
| ATOM | 4078 | CB | MET | 532 | 74.953 | 12.899 | 16.499 | 1.00 | 26.47 |
| ATOM | 4079 | CG | MET | 532 | 76.267 | 12.125 | 16.601 | 1.00 | 22.25 |
| ATOM | 4080 | SD | MET | 532 | 77.406 | 12.610 | 15.286 | 1.00 | 30.32 |
| ATOM | 4081 | CE | MET | 532 | 77.613 | 14.366 | 15.661 | 1.00 | 20.92 |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4082 | C | MET | 532 | 74.339 | 12.328 | 18.832 | 1.00 | 27.87 | |
| ATOM | 4083 | O | MET | 532 | 74.640 | 11.267 | 19.364 | 1.00 | 30.31 | |
| ATOM | 4084 | N | GLU | 533 | 74.439 | 13.497 | 19.442 | 1.00 | 27.08 | |
| ATOM | 4086 | CA | GLU | 533 | 74.906 | 13.594 | 20.802 | 1.00 | 28.50 | |
| ATOM | 4087 | CB | GLU | 533 | 75.071 | 15.064 | 21.177 | 1.00 | 29.09 | |
| ATOM | 4088 | CG | GLU | 533 | 76.216 | 15.745 | 20.433 | 1.00 | 28.90 | |
| ATOM | 4089 | CD | GLU | 533 | 77.564 | 15.070 | 20.661 | 1.00 | 31.08 | |
| ATOM | 4090 | OE1 | GLU | 533 | 78.001 | 14.969 | 21.823 | 1.00 | 34.15 | |
| ATOM | 4091 | OE2 | GLU | 533 | 78.202 | 14.643 | 19.678 | 1.00 | 33.60 | |
| ATOM | 4092 | C | GLU | 533 | 73.981 | 12.850 | 21.774 | 1.00 | 29.91 | |
| ATOM | 4093 | O | GLU | 533 | 74.455 | 12.093 | 22.637 | 1.00 | 29.73 | |
| ATOM | 4094 | N | MET | 534 | 72.670 | 13.014 | 21.588 | 1.00 | 29.70 | |
| ATOM | 4096 | CA | MET | 534 | 71.692 | 12.346 | 22.444 | 1.00 | 27.97 | |
| ATOM | 4097 | CB | MET | 534 | 70.258 | 12.751 | 22.082 | 1.00 | 28.95 | |
| ATOM | 4098 | CG | MET | 534 | 69.311 | 12.594 | 23.278 | 0.50 | 29.62 | PRT1 |
| ATOM | 4099 | SD | MET | 534 | 67.538 | 12.682 | 22.961 | 0.50 | 29.87 | PRT1 |
| ATOM | 4100 | CE | MET | 534 | 67.269 | 14.452 | 22.795 | 0.50 | 31.07 | PRT1 |
| ATOM | 4101 | C | MET | 534 | 71.855 | 10.821 | 22.362 | 1.00 | 28.36 | |
| ATOM | 4102 | O | MET | 534 | 71.833 | 10.143 | 23.386 | 1.00 | 27.02 | |
| ATOM | 4103 | N | MET | 535 | 72.048 | 10.297 | 21.151 | 1.00 | 26.96 | |
| ATOM | 4105 | CA | MET | 535 | 72.239 | 8.861 | 20.947 | 1.00 | 26.63 | |
| ATOM | 4106 | CB | MET | 535 | 72.347 | 8.521 | 19.456 | 1.00 | 24.67 | |
| ATOM | 4107 | CG | MET | 535 | 71.089 | 8.778 | 18.659 | 1.00 | 23.15 | |
| ATOM | 4108 | SD | MET | 535 | 71.160 | 8.062 | 17.011 | 1.00 | 24.57 | |
| ATOM | 4109 | CE | MET | 535 | 71.251 | 9.486 | 16.023 | 1.00 | 24.79 | |
| ATOM | 4110 | C | MET | 535 | 73.498 | 8.390 | 21.669 | 1.00 | 27.66 | |
| ATOM | 4111 | O | MET | 535 | 73.564 | 7.259 | 22.164 | 1.00 | 28.83 | |
| ATOM | 4112 | N | LYS | 536 | 74.515 | 9.246 | 21.698 | 1.00 | 29.13 | |
| ATOM | 4114 | CA | LYS | 536 | 75.757 | 8.918 | 22.392 | 1.00 | 30.50 | |
| ATOM | 4115 | CB | LYS | 536 | 76.812 | 9.985 | 22.131 | 1.00 | 29.15 | |
| ATOM | 4116 | CG | LYS | 536 | 77.499 | 9.883 | 20.802 | 1.00 | 27.71 | |
| ATOM | 4117 | CD | LYS | 536 | 78.377 | 11.100 | 20.615 | 1.00 | 28.12 | |
| ATOM | 4118 | CE | LYS | 536 | 79.085 | 11.096 | 19.279 | 1.00 | 26.89 | |
| ATOM | 4119 | NZ | LYS | 536 | 79.688 | 12.436 | 19.077 | 1.00 | 27.54 | |
| ATOM | 4123 | C | LYS | 536 | 75.480 | 8.836 | 23.892 | 1.00 | 31.92 | |
| ATOM | 4124 | O | LYS | 536 | 75.921 | 7.908 | 24.559 | 1.00 | 31.19 | |
| ATOM | 4125 | N | MET | 537 | 74.742 | 9.814 | 24.409 | 1.00 | 34.02 | |
| ATOM | 4127 | CA | MET | 537 | 74.384 | 9.881 | 25.822 | 1.00 | 36.35 | |
| ATOM | 4128 | CB | MET | 537 | 73.648 | 11.197 | 26.083 | 1.00 | 43.33 | |
| ATOM | 4129 | CG | MET | 537 | 73.096 | 11.376 | 27.507 | 1.00 | 54.60 | |
| ATOM | 4130 | SD | MET | 537 | 71.426 | 10.674 | 27.856 | 1.00 | 67.38 | |
| ATOM | 4131 | CE | MET | 537 | 71.684 | 9.813 | 29.440 | 1.00 | 62.03 | |
| ATOM | 4132 | C | MET | 537 | 73.507 | 8.705 | 26.253 | 1.00 | 34.53 | |
| ATOM | 4133 | O | MET | 537 | 73.744 | 8.069 | 27.275 | 1.00 | 36.76 | |
| ATOM | 4134 | N | ILE | 538 | 72.496 | 8.425 | 25.454 | 1.00 | 32.24 | |
| ATOM | 4136 | CA | ILE | 538 | 71.568 | 7.367 | 25.757 | 1.00 | 29.88 | |
| ATOM | 4137 | CB | ILE | 538 | 70.396 | 7.384 | 24.757 | 1.00 | 26.98 | |
| ATOM | 4138 | CG2 | ILE | 538 | 69.582 | 6.096 | 24.842 | 1.00 | 27.93 | |
| ATOM | 4139 | CG1 | ILE | 538 | 69.527 | 8.614 | 25.036 | 1.00 | 22.58 | |
| ATOM | 4140 | CD1 | ILE | 538 | 68.399 | 8.787 | 24.058 | 1.00 | 24.58 | |
| ATOM | 4141 | C | ILE | 538 | 72.236 | 6.006 | 25.804 | 1.00 | 31.83 | |
| ATOM | 4142 | O | ILE | 538 | 71.983 | 5.227 | 26.713 | 1.00 | 36.32 | |
| ATOM | 4143 | N | GLY | 539 | 73.102 | 5.718 | 24.848 | 1.00 | 32.45 | |
| ATOM | 4145 | CA | GLY | 539 | 73.744 | 4.422 | 24.850 | 1.00 | 32.13 | |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4146 | C | GLY | 539 | 72.974 | 3.380 | 24.056 | 1.00 | 33.83 |
| ATOM | 4147 | O | GLY | 539 | 71.876 | 3.654 | 23.530 | 1.00 | 33.75 |
| ATOM | 4148 | N | LYS | 540 | 73.539 | 2.173 | 24.010 | 1.00 | 33.36 |
| ATOM | 4150 | CA | LYS | 540 | 72.980 | 1.054 | 23.256 | 1.00 | 37.04 |
| ATOM | 4151 | CB | LYS | 540 | 74.110 | 0.181 | 22.709 | 1.00 | 39.21 |
| ATOM | 4152 | CG | LYS | 540 | 74.865 | 0.893 | 21.623 | 1.00 | 48.72 |
| ATOM | 4153 | CD | LYS | 540 | 75.818 | 0.009 | 20.850 | 1.00 | 56.84 |
| ATOM | 4154 | CE | LYS | 540 | 76.225 | 0.693 | 19.516 | 1.00 | 62.14 |
| ATOM | 4155 | NZ | LYS | 540 | 77.252 | -0.102 | 18.805 | 1.00 | 71.02 |
| ATOM | 4159 | C | LYS | 540 | 71.938 | 0.162 | 23.901 | 1.00 | 36.51 |
| ATOM | 4160 | O | LYS | 540 | 71.963 | -0.096 | 25.113 | 1.00 | 38.52 |
| ATOM | 4161 | N | HIS | 541 | 71.017 | -0.295 | 23.058 | 1.00 | 32.98 |
| ATOM | 4163 | CA | HIS | 541 | 69.963 | -1.230 | 23.424 | 1.00 | 31.20 |
| ATOM | 4164 | CB | HIS | 541 | 68.779 | -0.561 | 24.095 | 1.00 | 30.35 |
| ATOM | 4165 | CG | HIS | 541 | 67.815 | -1.540 | 24.694 | 1.00 | 32.56 |
| ATOM | 4166 | CD2 | HIS | 541 | 67.737 | -2.058 | 25.941 | 1.00 | 32.45 |
| ATOM | 4167 | ND1 | HIS | 541 | 66.795 | -2.124 | 23.974 | 1.00 | 29.22 |
| ATOM | 4169 | CE1 | HIS | 541 | 66.134 | -2.965 | 24.753 | 1.00 | 31.56 |
| ATOM | 4170 | NE2 | HIS | 541 | 66.679 | -2.932 | 25.957 | 1.00 | 32.22 |
| ATOM | 4172 | C | HIS | 541 | 69.509 | -1.937 | 22.152 | 1.00 | 32.00 |
| ATOM | 4173 | O | HIS | 541 | 69.409 | -1.324 | 21.095 | 1.00 | 32.84 |
| ATOM | 4174 | N | LYS | 542 | 69.187 | -3.222 | 22.273 | 1.00 | 33.61 |
| ATOM | 4176 | CA | LYS | 542 | 68.786 | -4.061 | 21.154 | 1.00 | 31.54 |
| ATOM | 4177 | CB | LYS | 542 | 68.653 | -5.516 | 21.596 | 1.00 | 33.94 |
| ATOM | 4178 | CG | LYS | 542 | 68.322 | -6.451 | 20.437 | 1.00 | 42.34 |
| ATOM | 4179 | CD | LYS | 542 | 68.083 | -7.885 | 20.856 | 1.00 | 47.57 |
| ATOM | 4180 | CE | LYS | 542 | 67.634 | -8.726 | 19.658 | 1.00 | 52.70 |
| ATOM | 4181 | NZ | LYS | 542 | 67.402 | -10.146 | 20.023 | 1.00 | 59.51 |
| ATOM | 4185 | C | LYS | 542 | 67.495 | -3.611 | 20.487 | 1.00 | 29.57 |
| ATOM | 4186 | O | LYS | 542 | 67.268 | -3.884 | 19.305 | 1.00 | 27.99 |
| ATOM | 4187 | N | ASN | 543 | 66.649 | -2.931 | 21.253 | 1.00 | 28.32 |
| ATOM | 4189 | CA | ASN | 543 | 65.378 | -2.476 | 20.714 | 1.00 | 28.86 |
| ATOM | 4190 | CB | ASN | 543 | 64.231 | -2.947 | 21.601 | 1.00 | 29.33 |
| ATOM | 4191 | CG | ASN | 543 | 64.247 | -4.452 | 21.811 | 1.00 | 29.64 |
| ATOM | 4192 | OD1 | ASN | 543 | 64.437 | -4.926 | 22.930 | 1.00 | 33.86 |
| ATOM | 4193 | ND2 | ASN | 543 | 64.106 | -5.206 | 20.732 | 1.00 | 28.02 |
| ATOM | 4196 | C | ASN | 543 | 65.252 | -0.983 | 20.378 | 1.00 | 29.69 |
| ATOM | 4197 | O | ASN | 543 | 64.159 | -0.413 | 20.457 | 1.00 | 30.02 |
| ATOM | 4198 | N | ILE | 544 | 66.372 | -0.357 | 20.011 | 1.00 | 27.35 |
| ATOM | 4200 | CA | ILE | 544 | 66.382 | 1.046 | 19.593 | 1.00 | 25.95 |
| ATOM | 4201 | CB | ILE | 544 | 66.898 | 2.030 | 20.706 | 1.00 | 25.56 |
| ATOM | 4202 | CG2 | ILE | 544 | 66.148 | 1.819 | 22.037 | 1.00 | 21.06 |
| ATOM | 4203 | CG1 | ILE | 544 | 68.406 | 1.901 | 20.902 | 1.00 | 25.61 |
| ATOM | 4204 | CD1 | ILE | 544 | 68.952 | 2.818 | 21.976 | 1.00 | 25.89 |
| ATOM | 4205 | C | ILE | 544 | 67.341 | 1.083 | 18.399 | 1.00 | 25.97 |
| ATOM | 4206 | O | ILE | 544 | 68.126 | 0.152 | 18.227 | 1.00 | 25.69 |
| ATOM | 4207 | N | ILE | 545 | 67.226 | 2.095 | 17.537 | 1.00 | 27.27 |
| ATOM | 4209 | CA | ILE | 545 | 68.129 | 2.243 | 16.384 | 1.00 | 27.02 |
| ATOM | 4210 | CB | ILE | 545 | 67.541 | 3.194 | 15.307 | 1.00 | 27.30 |
| ATOM | 4211 | CG2 | ILE | 545 | 68.592 | 3.553 | 14.269 | 1.00 | 26.52 |
| ATOM | 4212 | CG1 | ILE | 545 | 66.309 | 2.570 | 14.638 | 1.00 | 22.63 |
| ATOM | 4213 | CD1 | ILE | 545 | 66.605 | 1.447 | 13.665 | 1.00 | 17.57 |
| ATOM | 4214 | C | ILE | 545 | 69.383 | 2.873 | 16.979 | 1.00 | 28.55 |
| ATOM | 4215 | O | ILE | 545 | 69.346 | 4.014 | 17.451 | 1.00 | 29.47 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4216 | N | ASN | 546 | 70.482 | 2.123 | 16.965 | 1.00 | 30.90 |
| ATOM | 4218 | CA | ASN | 546 | 71.748 | 2.564 | 17.560 | 1.00 | 29.56 |
| ATOM | 4219 | CB | ASN | 546 | 72.497 | 1.365 | 18.159 | 1.00 | 26.32 |
| ATOM | 4220 | CG | ASN | 546 | 71.732 | 0.695 | 19.281 | 1.00 | 23.81 |
| ATOM | 4221 | OD1 | ASN | 546 | 71.580 | 1.252 | 20.362 | 1.00 | 27.34 |
| ATOM | 4222 | ND2 | ASN | 546 | 71.267 | -0.515 | 19.039 | 1.00 | 23.49 |
| ATOM | 4225 | C | ASN | 546 | 72.700 | 3.330 | 16.653 | 1.00 | 30.99 |
| ATOM | 4226 | O | ASN | 546 | 72.679 | 3.169 | 15.430 | 1.00 | 30.98 |
| ATOM | 4227 | N | LEU | 547 | 73.543 | 4.148 | 17.286 | 1.00 | 32.29 |
| ATOM | 4229 | CA | LEU | 547 | 74.570 | 4.948 | 16.610 | 1.00 | 30.93 |
| ATOM | 4230 | CB | LEU | 547 | 75.043 | 6.076 | 17.542 | 1.00 | 25.97 |
| ATOM | 4231 | CG | LEU | 547 | 76.075 | 7.088 | 17.021 | 1.00 | 22.12 |
| ATOM | 4232 | CD1 | LEU | 547 | 75.553 | 7.815 | 15.765 | 1.00 | 22.10 |
| ATOM | 4233 | CD2 | LEU | 547 | 76.415 | 8.089 | 18.112 | 1.00 | 18.67 |
| ATOM | 4234 | C | LEU | 547 | 75.756 | 4.039 | 16.264 | 1.00 | 30.70 |
| ATOM | 4235 | O | LEU | 547 | 76.284 | 3.361 | 17.137 | 1.00 | 34.46 |
| ATOM | 4236 | N | LEU | 548 | 76.141 | 3.993 | 14.992 | 1.00 | 30.97 |
| ATOM | 4238 | CA | LEU | 548 | 77.262 | 3.165 | 14.562 | 1.00 | 30.73 |
| ATOM | 4239 | CB | LEU | 548 | 76.929 | 2.406 | 13.281 | 1.00 | 29.24 |
| ATOM | 4240 | CG | LEU | 548 | 75.788 | 1.394 | 13.371 | 1.00 | 28.77 |
| ATOM | 4241 | CD1 | LEU | 548 | 75.924 | 0.460 | 12.209 | 1.00 | 26.55 |
| ATOM | 4242 | CD2 | LEU | 548 | 75.839 | 0.616 | 14.683 | 1.00 | 23.48 |
| ATOM | 4243 | C | LEU | 548 | 78.522 | 3.982 | 14.347 | 1.00 | 33.00 |
| ATOM | 4244 | O | LEU | 548 | 79.640 | 3.500 | 14.558 | 1.00 | 35.92 |
| ATOM | 4245 | N | GLY | 549 | 78.351 | 5.215 | 13.901 | 1.00 | 32.52 |
| ATOM | 4247 | CA | GLY | 549 | 79.503 | 6.051 | 13.673 | 1.00 | 32.76 |
| ATOM | 4248 | C | GLY | 549 | 79.092 | 7.411 | 13.180 | 1.00 | 33.72 |
| ATOM | 4249 | O | GLY | 549 | 77.895 | 7.707 | 13.092 | 1.00 | 35.01 |
| ATOM | 4250 | N | ALA | 550 | 80.089 | 8.226 | 12.840 | 1.00 | 33.47 |
| ATOM | 4252 | CA | ALA | 550 | 79.848 | 9.566 | 12.337 | 1.00 | 30.69 |
| ATOM | 4253 | CB | ALA | 550 | 79.555 | 10.509 | 13.497 | 1.00 | 28.66 |
| ATOM | 4254 | C | ALA | 550 | 81.022 | 10.099 | 11.523 | 1.00 | 30.41 |
| ATOM | 4255 | O | ALA | 550 | 82.181 | 9.780 | 11.808 | 1.00 | 25.13 |
| ATOM | 4256 | N | CYS | 551 | 80.695 | 10.817 | 10.446 | 1.00 | 30.29 |
| ATOM | 4258 | CA | CYS | 551 | 81.675 | 11.490 | 9.584 | 1.00 | 28.44 |
| ATOM | 4259 | CB | CYS | 551 | 81.432 | 11.214 | 8.096 | 1.00 | 27.25 |
| ATOM | 4260 | SG | CYS | 551 | 81.639 | 9.508 | 7.566 | 1.00 | 28.89 |
| ATOM | 4261 | C | CYS | 551 | 81.337 | 12.950 | 9.883 | 1.00 | 27.07 |
| ATOM | 4262 | O | CYS | 551 | 80.293 | 13.441 | 9.467 | 1.00 | 29.86 |
| ATOM | 4263 | N | THR | 552 | 82.184 | 13.616 | 10.658 | 1.00 | 25.10 |
| ATOM | 4265 | CA | THR | 552 | 81.952 | 14.997 | 11.047 | 1.00 | 24.37 |
| ATOM | 4266 | CB | THR | 552 | 81.959 | 15.091 | 12.569 | 1.00 | 27.67 |
| ATOM | 4267 | OG1 | THR | 552 | 83.271 | 14.760 | 13.052 | 1.00 | 26.11 |
| ATOM | 4269 | CG2 | THR | 552 | 80.951 | 14.120 | 13.164 | 1.00 | 30.41 |
| ATOM | 4270 | C | THR | 552 | 83.003 | 15.980 | 10.557 | 1.00 | 24.51 |
| ATOM | 4271 | O | THR | 552 | 82.804 | 17.194 | 10.604 | 1.00 | 21.56 |
| ATOM | 4272 | N | GLN | 553 | 84.151 | 15.441 | 10.162 | 1.00 | 27.13 |
| ATOM | 4274 | CA | GLN | 553 | 85.284 | 16.243 | 9.710 | 1.00 | 26.64 |
| ATOM | 4275 | CB | GLN | 553 | 86.592 | 15.679 | 10.283 | 1.00 | 25.24 |
| ATOM | 4276 | CG | GLN | 553 | 86.641 | 15.561 | 11.809 | 1.00 | 22.38 |
| ATOM | 4277 | CD | GLN | 553 | 86.464 | 16.897 | 12.515 | 1.00 | 24.04 |
| ATOM | 4278 | OE1 | GLN | 553 | 87.267 | 17.815 | 12.344 | 1.00 | 31.50 |
| ATOM | 4279 | NE2 | GLN | 553 | 85.403 | 17.017 | 13.304 | 1.00 | 21.59 |
| ATOM | 4282 | C | GLN | 553 | 85.384 | 16.276 | 8.206 | 1.00 | 28.02 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4283 | O | GLN | 553 | 85.069 | 15.293 | 7.537 | 1.00 | 30.20 |
| ATOM | 4284 | N | ASP | 554 | 85.794 | 17.430 | 7.695 | 1.00 | 28.08 |
| ATOM | 4286 | CA | ASP | 554 | 86.000 | 17.652 | 6.263 | 1.00 | 30.14 |
| ATOM | 4287 | CB | ASP | 554 | 87.330 | 17.034 | 5.833 | 1.00 | 29.82 |
| ATOM | 4288 | CG | ASP | 554 | 88.451 | 17.470 | 6.707 | 1.00 | 31.79 |
| ATOM | 4289 | OD1 | ASP | 554 | 88.699 | 18.666 | 6.767 | 1.00 | 36.45 |
| ATOM | 4290 | OD2 | ASP | 554 | 89.066 | 16.623 | 7.364 | 1.00 | 33.06 |
| ATOM | 4291 | C | ASP | 554 | 84.895 | 17.217 | 5.317 | 1.00 | 29.52 |
| ATOM | 4292 | O | ASP | 554 | 85.128 | 16.411 | 4.424 | 1.00 | 33.67 |
| ATOM | 4293 | N | GLY | 555 | 83.709 | 17.793 | 5.488 | 1.00 | 29.02 |
| ATOM | 4295 | CA | GLY | 555 | 82.586 | 17.476 | 4.621 | 1.00 | 26.05 |
| ATOM | 4296 | C | GLY | 555 | 81.286 | 17.447 | 5.405 | 1.00 | 23.80 |
| ATOM | 4297 | O | GLY | 555 | 81.269 | 17.751 | 6.597 | 1.00 | 24.09 |
| ATOM | 4298 | N | PRO | 556 | 80.175 | 17.117 | 4.740 | 1.00 | 23.29 |
| ATOM | 4299 | CD | PRO | 556 | 80.094 | 16.804 | 3.304 | 1.00 | 18.93 |
| ATOM | 4300 | CA | PRO | 556 | 78.860 | 17.045 | 5.378 | 1.00 | 23.45 |
| ATOM | 4301 | CB | PRO | 556 | 77.943 | 16.643 | 4.226 | 1.00 | 22.35 |
| ATOM | 4302 | CG | PRO | 556 | 78.889 | 15.931 | 3.261 | 1.00 | 24.94 |
| ATOM | 4303 | C | PRO | 556 | 78.806 | 16.019 | 6.503 | 1.00 | 26.66 |
| ATOM | 4304 | O | PRO | 556 | 79.488 | 14.984 | 6.464 | 1.00 | 27.76 |
| ATOM | 4305 | N | LEU | 557 | 78.006 | 16.324 | 7.522 | 1.00 | 29.14 |
| ATOM | 4307 | CA | LEU | 557 | 77.842 | 15.440 | 8.676 | 1.00 | 30.83 |
| ATOM | 4308 | CB | LEU | 557 | 77.173 | 16.181 | 9.842 | 1.00 | 28.40 |
| ATOM | 4309 | CG | LEU | 557 | 76.775 | 15.393 | 11.097 | 1.00 | 22.93 |
| ATOM | 4310 | CD1 | LEU | 557 | 77.989 | 14.897 | 11.835 | 1.00 | 23.02 |
| ATOM | 4311 | CD2 | LEU | 557 | 75.970 | 16.285 | 11.984 | 1.00 | 23.53 |
| ATOM | 4312 | C | LEU | 557 | 77.028 | 14.200 | 8.321 | 1.00 | 31.04 |
| ATOM | 4313 | O | LEU | 557 | 75.968 | 14.293 | 7.694 | 1.00 | 31.89 |
| ATOM | 4314 | N | TYR | 558 | 77.552 | 13.041 | 8.700 | 1.00 | 29.88 |
| ATOM | 4316 | CA | TYR | 558 | 76.891 | 11.773 | 8.460 | 1.00 | 27.80 |
| ATOM | 4317 | CB | TYR | 558 | 77.741 | 10.878 | 7.562 | 1.00 | 28.04 |
| ATOM | 4318 | CG | TYR | 558 | 77.895 | 11.339 | 6.122 | 1.00 | 29.98 |
| ATOM | 4319 | CD1 | TYR | 558 | 78.843 | 10.751 | 5.289 | 1.00 | 31.81 |
| ATOM | 4320 | CE1 | TYR | 558 | 78.980 | 11.140 | 3.956 | 1.00 | 32.22 |
| ATOM | 4321 | CD2 | TYR | 558 | 77.086 | 12.335 | 5.584 | 1.00 | 31.50 |
| ATOM | 4322 | CE2 | TYR | 558 | 77.214 | 12.729 | 4.256 | 1.00 | 31.57 |
| ATOM | 4323 | CZ | TYR | 558 | 78.166 | 12.125 | 3.449 | 1.00 | 32.04 |
| ATOM | 4324 | OH | TYR | 558 | 78.317 | 12.511 | 2.134 | 1.00 | 33.34 |
| ATOM | 4326 | C | TYR | 558 | 76.715 | 11.099 | 9.809 | 1.00 | 27.34 |
| ATOM | 4327 | O | TYR | 558 | 77.678 | 10.937 | 10.558 | 1.00 | 25.80 |
| ATOM | 4328 | N | VAL | 559 | 75.464 | 10.798 | 10.147 | 1.00 | 28.06 |
| ATOM | 4330 | CA | VAL | 559 | 75.118 | 10.118 | 11.394 | 1.00 | 26.67 |
| ATOM | 4331 | CB | VAL | 559 | 73.930 | 10.816 | 12.129 | 1.00 | 26.22 |
| ATOM | 4332 | CG1 | VAL | 559 | 73.590 | 10.079 | 13.425 | 1.00 | 22.58 |
| ATOM | 4333 | CG2 | VAL | 559 | 74.298 | 12.278 | 12.440 | 1.00 | 23.09 |
| ATOM | 4334 | C | VAL | 559 | 74.745 | 8.715 | 10.943 | 1.00 | 24.32 |
| ATOM | 4335 | O | VAL | 559 | 73.665 | 8.464 | 10.412 | 1.00 | 26.37 |
| ATOM | 4336 | N | ILE | 560 | 75.689 | 7.815 | 11.095 | 1.00 | 23.63 |
| ATOM | 4338 | CA | ILE | 560 | 75.514 | 6.448 | 10.664 | 1.00 | 24.67 |
| ATOM | 4339 | CB | ILE | 560 | 76.901 | 5.859 | 10.299 | 1.00 | 24.62 |
| ATOM | 4340 | CG2 | ILE | 560 | 76.753 | 4.507 | 9.646 | 1.00 | 30.13 |
| ATOM | 4341 | CG1 | ILE | 560 | 77.627 | 6.810 | 9.326 | 1.00 | 21.87 |
| ATOM | 4342 | CD1 | ILE | 560 | 79.114 | 6.538 | 9.162 | 1.00 | 22.25 |
| ATOM | 4343 | C | ILE | 560 | 74.814 | 5.621 | 11.737 | 1.00 | 27.30 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4344 | O | ILE | 560 | 75.306 | 5.505 | 12.865 | 1.00 | 28.80 |
| ATOM | 4345 | N | VAL | 561 | 73.641 | 5.090 | 11.406 | 1.00 | 26.80 |
| ATOM | 4347 | CA | VAL | 561 | 72.894 | 4.272 | 12.352 | 1.00 | 26.16 |
| ATOM | 4348 | CB | VAL | 561 | 71.572 | 4.953 | 12.810 | 1.00 | 24.10 |
| ATOM | 4349 | CG1 | VAL | 561 | 71.866 | 6.208 | 13.599 | 1.00 | 24.11 |
| ATOM | 4350 | CG2 | VAL | 561 | 70.676 | 5.254 | 11.625 | 1.00 | 21.97 |
| ATOM | 4351 | C | VAL | 561 | 72.572 | 2.901 | 11.761 | 1.00 | 27.98 |
| ATOM | 4352 | O | VAL | 561 | 72.853 | 2.632 | 10.584 | 1.00 | 26.49 |
| ATOM | 4353 | N | GLU | 562 | 71.998 | 2.039 | 12.599 | 1.00 | 28.86 |
| ATOM | 4355 | CA | GLU | 562 | 71.605 | 0.685 | 12.219 | 1.00 | 28.23 |
| ATOM | 4356 | CB | GLU | 562 | 71.090 | -0.068 | 13.440 | 1.00 | 25.86 |
| ATOM | 4357 | CG | GLU | 562 | 72.170 | -0.392 | 14.424 | 1.00 | 27.04 |
| ATOM | 4358 | CD | GLU | 562 | 71.641 | -0.969 | 15.714 | 1.00 | 28.37 |
| ATOM | 4359 | OE1 | GLU | 562 | 72.389 | -1.714 | 16.372 | 1.00 | 33.36 |
| ATOM | 4360 | OE2 | GLU | 562 | 70.491 | -0.665 | 16.092 | 1.00 | 31.60 |
| ATOM | 4361 | C | GLU | 562 | 70.529 | 0.720 | 11.171 | 1.00 | 29.67 |
| ATOM | 4362 | O | GLU | 562 | 69.581 | 1.489 | 11.287 | 1.00 | 32.53 |
| ATOM | 4363 | N | TYR | 563 | 70.666 | -0.126 | 10.162 | 1.00 | 30.70 |
| ATOM | 4365 | CA | TYR | 563 | 69.699 | -0.209 | 9.083 | 1.00 | 30.65 |
| ATOM | 4366 | CB | TYR | 563 | 70.419 | -0.621 | 7.801 | 1.00 | 30.83 |
| ATOM | 4367 | CG | TYR | 563 | 69.510 | -0.905 | 6.633 | 1.00 | 32.10 |
| ATOM | 4368 | CD1 | TYR | 563 | 68.545 | 0.018 | 6.236 | 1.00 | 33.24 |
| ATOM | 4369 | CE1 | TYR | 563 | 67.715 | -0.227 | 5.160 | 1.00 | 34.65 |
| ATOM | 4370 | CD2 | TYR | 563 | 69.609 | -2.098 | 5.922 | 1.00 | 31.04 |
| ATOM | 4371 | CE2 | TYR | 563 | 68.779 | -2.353 | 4.838 | 1.00 | 33.12 |
| ATOM | 4372 | CZ | TYR | 563 | 67.831 | -1.413 | 4.470 | 1.00 | 34.22 |
| ATOM | 4373 | OH | TYR | 563 | 67.002 | -1.650 | 3.400 | 1.00 | 34.76 |
| ATOM | 4375 | C | TYR | 563 | 68.592 | -1.223 | 9.406 | 1.00 | 34.39 |
| ATOM | 4376 | O | TYR | 563 | 68.855 | -2.325 | 9.884 | 1.00 | 34.87 |
| ATOM | 4377 | N | ALA | 564 | 67.356 | -0.861 | 9.091 | 1.00 | 35.49 |
| ATOM | 4379 | CA | ALA | 564 | 66.212 | -1.726 | 9.324 | 1.00 | 35.41 |
| ATOM | 4380 | CB | ALA | 564 | 65.213 | -1.000 | 10.210 | 1.00 | 35.93 |
| ATOM | 4381 | C | ALA | 564 | 65.585 | -2.056 | 7.962 | 1.00 | 37.19 |
| ATOM | 4382 | O | ALA | 564 | 64.789 | -1.276 | 7.434 | 1.00 | 38.08 |
| ATOM | 4383 | N | SER | 565 | 65.931 | -3.211 | 7.401 | 1.00 | 37.14 |
| ATOM | 4385 | CA | SER | 565 | 65.433 | -3.616 | 6.080 | 1.00 | 36.83 |
| ATOM | 4386 | CB | SER | 565 | 66.151 | -4.881 | 5.614 | 1.00 | 35.24 |
| ATOM | 4387 | OG | SER | 565 | 66.105 | -5.873 | 6.619 | 1.00 | 34.96 |
| ATOM | 4389 | C | SER | 565 | 63.932 | -3.782 | 5.886 | 1.00 | 38.65 |
| ATOM | 4390 | O | SER | 565 | 63.428 | -3.617 | 4.760 | 1.00 | 37.80 |
| ATOM | 4391 | N | LYS | 566 | 63.212 | -4.077 | 6.964 | 1.00 | 38.96 |
| ATOM | 4393 | CA | LYS | 566 | 61.772 | -4.271 | 6.851 | 1.00 | 37.83 |
| ATOM | 4394 | CB | LYS | 566 | 61.357 | -5.495 | 7.655 | 1.00 | 39.07 |
| ATOM | 4395 | CG | LYS | 566 | 61.954 | -6.765 | 7.078 | 1.00 | 43.73 |
| ATOM | 4396 | CD | LYS | 566 | 61.813 | -7.950 | 7.996 | 1.00 | 47.07 |
| ATOM | 4397 | CE | LYS | 566 | 62.258 | -9.216 | 7.299 | 1.00 | 47.77 |
| ATOM | 4398 | NZ | LYS | 566 | 62.361 | -10.326 | 8.278 | 1.00 | 51.48 |
| ATOM | 4402 | C | LYS | 566 | 60.899 | -3.050 | 7.165 | 1.00 | 37.53 |
| ATOM | 4403 | O | LYS | 566 | 59.702 | -3.180 | 7.442 | 1.00 | 38.55 |
| ATOM | 4404 | N | GLY | 567 | 61.496 | -1.866 | 7.066 | 1.00 | 35.23 |
| ATOM | 4406 | CA | GLY | 567 | 60.788 | -0.627 | 7.305 | 1.00 | 33.64 |
| ATOM | 4407 | C | GLY | 567 | 60.120 | -0.485 | 8.656 | 1.00 | 33.24 |
| ATOM | 4408 | O | GLY | 567 | 60.518 | -1.133 | 9.627 | 1.00 | 33.80 |
| ATOM | 4409 | N | ASN | 568 | 59.120 | 0.389 | 8.716 | 1.00 | 31.65 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4411 | CA | ASN | 568 | 58.407 | 0.623 | 9.952 | 1.00 | 33.38 |
| ATOM | 4412 | CB | ASN | 568 | 57.831 | 2.055 | 10.025 | 1.00 | 37.10 |
| ATOM | 4413 | CG | ASN | 568 | 56.624 | 2.272 | 9.116 | 1.00 | 37.78 |
| ATOM | 4414 | OD1 | ASN | 568 | 55.552 | 1.708 | 9.337 | 1.00 | 41.15 |
| ATOM | 4415 | ND2 | ASN | 568 | 56.780 | 3.147 | 8.124 | 1.00 | 35.74 |
| ATOM | 4418 | C | ASN | 568 | 57.357 | -0.435 | 10.263 | 1.00 | 33.33 |
| ATOM | 4419 | O | ASN | 568 | 56.917 | -1.178 | 9.384 | 1.00 | 32.54 |
| ATOM | 4420 | N | LEU | 569 | 56.971 | -0.490 | 11.532 | 1.00 | 33.35 |
| ATOM | 4422 | CA | LEU | 569 | 56.004 | -1.455 | 12.040 | 1.00 | 32.38 |
| ATOM | 4423 | CB | LEU | 569 | 55.838 | -1.263 | 13.552 | 1.00 | 27.50 |
| ATOM | 4424 | CG | LEU | 569 | 54.954 | -2.259 | 14.291 | 1.00 | 26.34 |
| ATOM | 4425 | CD1 | LEU | 569 | 55.452 | -3.671 | 14.007 | 1.00 | 24.19 |
| ATOM | 4426 | CD2 | LEU | 569 | 54.968 | -1.951 | 15.787 | 1.00 | 21.44 |
| ATOM | 4427 | C | LEU | 569 | 54.641 | -1.433 | 11.355 | 1.00 | 33.35 |
| ATOM | 4428 | O | LEU | 569 | 54.060 | -2.484 | 11.095 | 1.00 | 34.99 |
| ATOM | 4429 | N | ARG | 570 | 54.130 | -0.239 | 11.083 | 1.00 | 34.36 |
| ATOM | 4431 | CA | ARG | 570 | 52.827 | -0.091 | 10.445 | 1.00 | 36.82 |
| ATOM | 4432 | CB | ARG | 570 | 52.548 | 1.393 | 10.188 | 1.00 | 37.28 |
| ATOM | 4433 | CG | ARG | 570 | 51.210 | 1.689 | 9.539 | 1.00 | 43.90 |
| ATOM | 4434 | CD | ARG | 570 | 51.212 | 3.099 | 8.967 | 1.00 | 50.39 |
| ATOM | 4435 | NE | ARG | 570 | 52.273 | 3.268 | 7.973 | 1.00 | 54.99 |
| ATOM | 4437 | CZ | ARG | 570 | 53.075 | 4.328 | 7.887 | 1.00 | 54.96 |
| ATOM | 4438 | NH1 | ARG | 570 | 52.947 | 5.343 | 8.735 | 1.00 | 54.71 |
| ATOM | 4441 | NH2 | ARG | 570 | 54.030 | 4.357 | 6.966 | 1.00 | 56.12 |
| ATOM | 4444 | C | ARG | 570 | 52.818 | -0.877 | 9.133 | 1.00 | 36.53 |
| ATOM | 4445 | O | ARG | 570 | 51.968 | -1.737 | 8.909 | 1.00 | 34.68 |
| ATOM | 4446 | N | GLU | 571 | 53.830 | -0.611 | 8.320 | 1.00 | 37.14 |
| ATOM | 4448 | CA | GLU | 571 | 53.994 | -1.253 | 7.031 | 1.00 | 37.94 |
| ATOM | 4449 | CB | GLU | 571 | 55.126 | -0.558 | 6.274 | 1.00 | 39.71 |
| ATOM | 4450 | CG | GLU | 571 | 54.834 | 0.916 | 6.062 | 1.00 | 44.69 |
| ATOM | 4451 | CD | GLU | 571 | 55.934 | 1.665 | 5.346 | 1.00 | 52.22 |
| ATOM | 4452 | OE1 | GLU | 571 | 57.098 | 1.196 | 5.358 | 1.00 | 54.87 |
| ATOM | 4453 | OE2 | GLU | 571 | 55.629 | 2.743 | 4.777 | 1.00 | 56.37 |
| ATOM | 4454 | C | GLU | 571 | 54.258 | -2.744 | 7.164 | 1.00 | 36.53 |
| ATOM | 4455 | O | GLU | 571 | 53.692 | -3.550 | 6.426 | 1.00 | 36.35 |
| ATOM | 4456 | N | TYR | 572 | 55.105 | -3.105 | 8.120 | 1.00 | 35.77 |
| ATOM | 4458 | CA | TYR | 572 | 55.456 | -4.499 | 8.371 | 1.00 | 36.28 |
| ATOM | 4459 | CB | TYR | 572 | 56.446 | -4.555 | 9.534 | 1.00 | 30.27 |
| ATOM | 4460 | CG | TYR | 572 | 56.859 | -5.925 | 10.006 | 1.00 | 31.65 |
| ATOM | 4461 | CD1 | TYR | 572 | 57.889 | -6.626 | 9.371 | 1.00 | 29.40 |
| ATOM | 4462 | CE1 | TYR | 572 | 58.354 | -7.839 | 9.883 | 1.00 | 29.32 |
| ATOM | 4463 | CD2 | TYR | 572 | 56.292 | -6.480 | 11.161 | 1.00 | 35.17 |
| ATOM | 4464 | CE2 | TYR | 572 | 56.749 | -7.696 | 11.680 | 1.00 | 33.08 |
| ATOM | 4465 | CZ | TYR | 572 | 57.780 | -8.366 | 11.038 | 1.00 | 35.15 |
| ATOM | 4466 | OH | TYR | 572 | 58.234 | -9.559 | 11.558 | 1.00 | 36.91 |
| ATOM | 4468 | C | TYR | 572 | 54.189 | -5.321 | 8.672 | 1.00 | 37.70 |
| ATOM | 4469 | O | TYR | 572 | 53.942 | -6.369 | 8.068 | 1.00 | 36.82 |
| ATOM | 4470 | N | LEU | 573 | 53.368 | -4.799 | 9.576 | 1.00 | 37.64 |
| ATOM | 4472 | CA | LEU | 573 | 52.126 | -5.442 | 9.970 | 1.00 | 36.03 |
| ATOM | 4473 | CB | LEU | 573 | 51.497 | -4.659 | 11.122 | 1.00 | 36.17 |
| ATOM | 4474 | CG | LEU | 573 | 52.257 | -4.641 | 12.445 | 1.00 | 36.39 |
| ATOM | 4475 | CD1 | LEU | 573 | 51.590 | -3.665 | 13.412 | 1.00 | 36.17 |
| ATOM | 4476 | CD2 | LEU | 573 | 52.311 | -6.042 | 13.032 | 1.00 | 32.13 |
| ATOM | 4477 | C | LEU | 573 | 51.117 | -5.562 | 8.822 | 1.00 | 36.33 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4478 | O | LEU | 573 | 50.477 | -6.596 | 8.649 | 1.00 | 35.19 |
| ATOM | 4479 | N | GLN | 574 | 50.975 | -4.502 | 8.038 | 1.00 | 37.66 |
| ATOM | 4481 | CA | GLN | 574 | 50.024 | -4.514 | 6.936 | 1.00 | 41.78 |
| ATOM | 4482 | CB | GLN | 574 | 49.798 | -3.103 | 6.413 | 1.00 | 43.82 |
| ATOM | 4483 | CG | GLN | 574 | 48.898 | -2.273 | 7.264 | 1.00 | 45.42 |
| ATOM | 4484 | CD | GLN | 574 | 48.871 | -0.850 | 6.801 | 1.00 | 49.56 |
| ATOM | 4485 | OE1 | GLN | 574 | 49.456 | -0.506 | 5.772 | 1.00 | 52.22 |
| ATOM | 4486 | NE2 | GLN | 574 | 48.207 | 0.001 | 7.565 | 1.00 | 54.86 |
| ATOM | 4489 | C | GLN | 574 | 50.401 | -5.427 | 5.783 | 1.00 | 42.89 |
| ATOM | 4490 | O | GLN | 574 | 49.532 | -5.898 | 5.042 | 1.00 | 46.15 |
| ATOM | 4491 | N | ALA | 575 | 51.695 | -5.646 | 5.599 | 1.00 | 42.39 |
| ATOM | 4493 | CA | ALA | 575 | 52.165 | -6.516 | 4.532 | 1.00 | 40.19 |
| ATOM | 4494 | CB | ALA | 575 | 53.597 | -6.165 | 4.170 | 1.00 | 40.68 |
| ATOM | 4495 | C | ALA | 575 | 52.088 | -7.970 | 4.971 | 1.00 | 40.49 |
| ATOM | 4496 | O | ALA | 575 | 52.437 | -8.867 | 4.210 | 1.00 | 43.34 |
| ATOM | 4497 | N | ARG | 576 | 51.630 | -8.197 | 6.202 | 1.00 | 38.76 |
| ATOM | 4499 | CA | ARG | 576 | 51.538 | -9.542 | 6.761 | 1.00 | 38.44 |
| ATOM | 4500 | CB | ARG | 576 | 52.600 | -9.708 | 7.846 | 1.00 | 34.26 |
| ATOM | 4501 | CG | ARG | 576 | 53.991 | -9.609 | 7.284 | 1.00 | 37.16 |
| ATOM | 4502 | CD | ARG | 576 | 55.052 | -9.625 | 8.356 | 1.00 | 36.38 |
| ATOM | 4503 | NE | ARG | 576 | 56.384 | -9.663 | 7.760 | 1.00 | 36.98 |
| ATOM | 4505 | CZ | ARG | 576 | 56.897 | -8.714 | 6.983 | 1.00 | 38.62 |
| ATOM | 4506 | NH1 | ARG | 576 | 56.204 | -7.618 | 6.689 | 1.00 | 41.41 |
| ATOM | 4509 | NH2 | ARG | 576 | 58.112 | -8.863 | 6.491 | 1.00 | 37.48 |
| ATOM | 4512 | C | ARG | 576 | 50.165 | -9.860 | 7.321 | 1.00 | 40.55 |
| ATOM | 4513 | O | ARG | 576 | 50.013 | -10.746 | 8.169 | 1.00 | 43.20 |
| ATOM | 4514 | N | ARG | 577 | 49.156 | -9.146 | 6.844 | 1.00 | 41.98 |
| ATOM | 4516 | CA | ARG | 577 | 47.794 | -9.372 | 7.309 | 1.00 | 43.12 |
| ATOM | 4517 | CB | ARG | 577 | 46.896 | -8.226 | 6.851 | 1.00 | 44.21 |
| ATOM | 4518 | CG | ARG | 577 | 47.206 | -6.910 | 7.525 | 1.00 | 45.21 |
| ATOM | 4519 | CD | ARG | 577 | 46.402 | -5.766 | 6.941 | 1.00 | 47.50 |
| ATOM | 4520 | NE | ARG | 577 | 46.172 | -4.734 | 7.948 | 1.00 | 47.58 |
| ATOM | 4522 | CZ | ARG | 577 | 45.447 | -3.641 | 7.752 | 1.00 | 47.63 |
| ATOM | 4523 | NH1 | ARG | 577 | 44.882 | -3.421 | 6.574 | 1.00 | 49.05 |
| ATOM | 4526 | NH2 | ARG | 577 | 45.256 | -2.789 | 8.747 | 1.00 | 49.88 |
| ATOM | 4529 | C | ARG | 577 | 47.241 | -10.715 | 6.821 | 1.00 | 43.10 |
| ATOM | 4530 | O | ARG | 577 | 47.297 | -11.015 | 5.627 | 1.00 | 43.86 |
| ATOM | 4531 | N | GLN | 594 | 53.448 | -13.666 | 7.976 | 1.00 | 64.97 |
| ATOM | 4533 | CA | GLN | 594 | 52.231 | -13.872 | 8.759 | 1.00 | 66.30 |
| ATOM | 4534 | CB | GLN | 594 | 51.419 | -15.042 | 8.200 | 1.00 | 67.44 |
| ATOM | 4535 | C | GLN | 594 | 52.582 | -14.116 | 10.224 | 1.00 | 66.02 |
| ATOM | 4536 | O | GLN | 594 | 53.162 | -15.145 | 10.583 | 1.00 | 67.47 |
| ATOM | 4537 | N | LEU | 595 | 52.218 | -13.151 | 11.058 | 1.00 | 62.86 |
| ATOM | 4539 | CA | LEU | 595 | 52.499 | -13.187 | 12.480 | 1.00 | 59.77 |
| ATOM | 4540 | CB | LEU | 595 | 52.597 | -11.751 | 12.987 | 1.00 | 59.35 |
| ATOM | 4541 | CG | LEU | 595 | 53.471 | -10.905 | 12.051 | 1.00 | 61.70 |
| ATOM | 4542 | CD1 | LEU | 595 | 53.307 | -9.427 | 12.322 | 1.00 | 64.61 |
| ATOM | 4543 | CD2 | LEU | 595 | 54.923 | -11.324 | 12.175 | 1.00 | 62.38 |
| ATOM | 4544 | C | LEU | 595 | 51.482 | -13.985 | 13.290 | 1.00 | 57.49 |
| ATOM | 4545 | O | LEU | 595 | 50.302 | -14.026 | 12.951 | 1.00 | 56.36 |
| ATOM | 4546 | N | SER | 596 | 51.969 | -14.647 | 14.338 | 1.00 | 55.62 |
| ATOM | 4548 | CA | SER | 596 | 51.134 | -15.447 | 15.222 | 1.00 | 54.72 |
| ATOM | 4549 | CB | SER | 596 | 51.905 | -16.669 | 15.721 | 1.00 | 55.13 |
| ATOM | 4550 | OG | SER | 596 | 52.871 | -16.309 | 16.698 | 1.00 | 54.98 |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4552 | C | SER | 596 | 50.723 | -14.597 | 16.415 | 1.00 | 54.73 | |
| ATOM | 4553 | O | SER | 596 | 51.348 | -13.579 | 16.704 | 1.00 | 53.29 | |
| ATOM | 4554 | N | SER | 597 | 49.704 | -15.051 | 17.137 | 1.00 | 55.09 | |
| ATOM | 4556 | CA | SER | 597 | 49.215 | -14.337 | 18.307 | 1.00 | 56.44 | |
| ATOM | 4557 | CB | SER | 597 | 48.178 | -15.185 | 19.044 | 1.00 | 59.14 | |
| ATOM | 4558 | OG | SER | 597 | 47.455 | -16.009 | 18.138 | 1.00 | 65.57 | |
| ATOM | 4560 | C | SER | 597 | 50.387 | -14.026 | 19.238 | 1.00 | 55.64 | |
| ATOM | 4561 | O | SER | 597 | 50.430 | -12.966 | 19.856 | 1.00 | 56.04 | |
| ATOM | 4562 | N | LYS | 598 | 51.345 | -14.948 | 19.315 | 1.00 | 54.91 | |
| ATOM | 4564 | CA | LYS | 598 | 52.528 | -14.773 | 20.161 | 1.00 | 54.25 | |
| ATOM | 4565 | CB | LYS | 598 | 53.287 | -16.096 | 20.311 | 1.00 | 54.23 | |
| ATOM | 4566 | CG | LYS | 598 | 54.236 | -16.138 | 21.494 | 1.00 | 55.12 | |
| ATOM | 4567 | CD | LYS | 598 | 55.009 | -17.448 | 21.523 | 1.00 | 59.41 | |
| ATOM | 4568 | CE | LYS | 598 | 55.711 | -17.679 | 22.858 | 1.00 | 58.10 | |
| ATOM | 4569 | NZ | LYS | 598 | 54.750 | -17.983 | 23.959 | 1.00 | 56.10 | |
| ATOM | 4573 | C | LYS | 598 | 53.439 | -13.716 | 19.536 | 1.00 | 52.32 | |
| ATOM | 4574 | O | LYS | 598 | 53.986 | -12.869 | 20.249 | 1.00 | 52.23 | |
| ATOM | 4575 | N | ASP | 599 | 53.573 | -13.768 | 18.208 | 1.00 | 47.57 | |
| ATOM | 4577 | CA | ASP | 599 | 54.389 | -12.818 | 17.466 | 1.00 | 45.47 | |
| ATOM | 4578 | CB | ASP | 599 | 54.324 | -13.101 | 15.959 | 1.00 | 49.05 | |
| ATOM | 4579 | CG | ASP | 599 | 55.245 | -14.238 | 15.525 | 1.00 | 54.16 | |
| ATOM | 4580 | OD1 | ASP | 599 | 56.242 | -14.503 | 16.223 | 1.00 | 61.34 | |
| ATOM | 4581 | OD2 | ASP | 599 | 54.992 | -14.863 | 14.471 | 1.00 | 55.80 | |
| ATOM | 4582 | C | ASP | 599 | 53.933 | -11.383 | 17.721 | 1.00 | 43.55 | |
| ATOM | 4583 | O | ASP | 599 | 54.762 | -10.491 | 17.895 | 1.00 | 44.34 | |
| ATOM | 4584 | N | LEU | 600 | 52.622 | -11.160 | 17.751 | 1.00 | 39.73 | |
| ATOM | 4586 | CA | LEU | 600 | 52.104 | -9.821 | 17.989 | 1.00 | 37.64 | |
| ATOM | 4587 | CB | LEU | 600 | 50.597 | -9.743 | 17.719 | 1.00 | 35.42 | |
| ATOM | 4588 | CG | LEU | 600 | 50.075 | -9.951 | 16.287 | 1.00 | 33.95 | |
| ATOM | 4589 | CD1 | LEU | 600 | 48.621 | -9.552 | 16.262 | 1.00 | 36.59 | |
| ATOM | 4590 | CD2 | LEU | 600 | 50.841 | -9.139 | 15.265 | 1.00 | 28.40 | |
| ATOM | 4591 | C | LEU | 600 | 52.429 | -9.347 | 19.402 | 1.00 | 38.24 | |
| ATOM | 4592 | O | LEU | 600 | 52.817 | -8.193 | 19.590 | 1.00 | 38.28 | |
| ATOM | 4593 | N | VAL | 601 | 52.305 | -10.235 | 20.391 | 1.00 | 38.77 | |
| ATOM | 4595 | CA | VAL | 601 | 52.610 | -9.855 | 21.772 | 1.00 | 38.87 | |
| ATOM | 4596 | CB | VAL | 601 | 52.121 | -10.906 | 22.812 | 1.00 | 38.03 | |
| ATOM | 4597 | CG1 | VAL | 601 | 52.150 | -10.303 | 24.223 | 1.00 | 36.21 | |
| ATOM | 4598 | CG2 | VAL | 601 | 50.710 | -11.332 | 22.504 | 1.00 | 39.07 | |
| ATOM | 4599 | C | VAL | 601 | 54.123 | -9.662 | 21.887 | 1.00 | 38.98 | |
| ATOM | 4600 | O | VAL | 601 | 54.601 | -8.757 | 22.580 | 1.00 | 39.93 | |
| ATOM | 4601 | N | SER | 602 | 54.861 | -10.488 | 21.155 | 1.00 | 37.35 | |
| ATOM | 4603 | CA | SER | 602 | 56.311 | -10.422 | 21.126 | 1.00 | 37.11 | |
| ATOM | 4604 | CB | SER | 602 | 56.853 | -11.469 | 20.154 | 1.00 | 39.38 | |
| ATOM | 4605 | OG | SER | 602 | 58.265 | -11.413 | 20.061 | 1.00 | 46.76 | |
| ATOM | 4607 | C | SER | 602 | 56.695 | -9.020 | 20.664 | 1.00 | 35.43 | |
| ATOM | 4608 | O | SER | 602 | 57.493 | -8.339 | 21.315 | 1.00 | 35.01 | |
| ATOM | 4609 | N | CYS | 603 | 56.091 | -8.586 | 19.561 | 1.00 | 33.42 | |
| ATOM | 4611 | CA | CYS | 603 | 56.329 | -7.254 | 19.015 | 1.00 | 32.18 | |
| ATOM | 4612 | CB | CYS | 603 | 55.449 | -7.035 | 17.790 | 1.00 | 32.38 | |
| ATOM | 4613 | SG | CYS | 603 | 55.440 | -5.365 | 17.123 | 0.50 | 35.11 | PRT1 |
| ATOM | 4614 | C | CYS | 603 | 56.074 | -6.167 | 20.059 | 1.00 | 31.20 | |
| ATOM | 4615 | O | CYS | 603 | 56.862 | -5.234 | 20.185 | 1.00 | 32.44 | |
| ATOM | 4616 | N | ALA | 604 | 55.001 | -6.321 | 20.828 | 1.00 | 29.74 | |
| ATOM | 4618 | CA | ALA | 604 | 54.640 | -5.363 | 21.872 | 1.00 | 32.26 | |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4619 | CB | ALA | 604 | 53.232 | -5.675 | 22.412 | 1.00 | 31.75 |
| ATOM | 4620 | C | ALA | 604 | 55.656 | -5.365 | 23.019 | 1.00 | 33.71 |
| ATOM | 4621 | O | ALA | 604 | 55.933 | -4.326 | 23.621 | 1.00 | 33.49 |
| ATOM | 4622 | N | TYR | 605 | 56.186 | -6.544 | 23.326 | 1.00 | 35.56 |
| ATOM | 4624 | CA | TYR | 605 | 57.176 | -6.709 | 24.388 | 1.00 | 35.49 |
| ATOM | 4625 | CB | TYR | 605 | 57.447 | -8.206 | 24.617 | 1.00 | 36.12 |
| ATOM | 4626 | CG | TYR | 605 | 58.562 | -8.495 | 25.591 | 1.00 | 34.75 |
| ATOM | 4627 | CD1 | TYR | 605 | 58.415 | -8.237 | 26.954 | 1.00 | 34.30 |
| ATOM | 4628 | CE1 | TYR | 605 | 59.444 | -8.499 | 27.853 | 1.00 | 36.26 |
| ATOM | 4629 | CD2 | TYR | 605 | 59.773 | -9.021 | 25.150 | 1.00 | 37.39 |
| ATOM | 4630 | CE2 | TYR | 605 | 60.812 | -9.288 | 26.040 | 1.00 | 37.81 |
| ATOM | 4631 | CZ | TYR | 605 | 60.641 | -9.027 | 27.388 | 1.00 | 38.34 |
| ATOM | 4632 | OH | TYR | 605 | 61.662 | -9.324 | 28.265 | 1.00 | 42.09 |
| ATOM | 4634 | C | TYR | 605 | 58.475 | -5.972 | 24.027 | 1.00 | 34.98 |
| ATOM | 4635 | O | TYR | 605 | 58.981 | -5.171 | 24.822 | 1.00 | 35.83 |
| ATOM | 4636 | N | GLN | 606 | 58.996 | -6.247 | 22.828 | 1.00 | 33.99 |
| ATOM | 4638 | CA | GLN | 606 | 60.218 | -5.620 | 22.315 | 1.00 | 33.60 |
| ATOM | 4639 | CB | GLN | 606 | 60.506 | -6.111 | 20.894 | 1.00 | 31.37 |
| ATOM | 4640 | CG | GLN | 606 | 60.858 | -7.584 | 20.786 | 1.00 | 32.05 |
| ATOM | 4641 | CD | GLN | 606 | 61.175 | -8.015 | 19.354 | 1.00 | 30.33 |
| ATOM | 4642 | OE1 | GLN | 606 | 62.145 | -7.558 | 18.754 | 1.00 | 30.84 |
| ATOM | 4643 | NE2 | GLN | 606 | 60.353 | -8.895 | 18.810 | 1.00 | 33.75 |
| ATOM | 4646 | C | GLN | 606 | 60.123 | -4.079 | 22.321 | 1.00 | 34.86 |
| ATOM | 4647 | O | GLN | 606 | 61.070 | -3.390 | 22.702 | 1.00 | 37.54 |
| ATOM | 4648 | N | VAL | 607 | 58.975 | -3.555 | 21.904 | 1.00 | 32.89 |
| ATOM | 4650 | CA | VAL | 607 | 58.748 | -2.114 | 21.883 | 1.00 | 30.80 |
| ATOM | 4651 | CB | VAL | 607 | 57.426 | -1.777 | 21.120 | 1.00 | 28.82 |
| ATOM | 4652 | CG1 | VAL | 607 | 57.121 | -0.299 | 21.191 | 1.00 | 25.36 |
| ATOM | 4653 | CG2 | VAL | 607 | 57.541 | -2.204 | 19.661 | 1.00 | 23.37 |
| ATOM | 4654 | C | VAL | 607 | 58.747 | -1.532 | 23.312 | 1.00 | 30.48 |
| ATOM | 4655 | O | VAL | 607 | 59.359 | -0.485 | 23.563 | 1.00 | 29.42 |
| ATOM | 4656 | N | ALA | 608 | 58.106 | -2.225 | 24.255 | 1.00 | 30.07 |
| ATOM | 4658 | CA | ALA | 608 | 58.064 | -1.761 | 25.646 | 1.00 | 30.14 |
| ATOM | 4659 | CB | ALA | 608 | 57.027 | -2.548 | 26.452 | 1.00 | 28.49 |
| ATOM | 4660 | C | ALA | 608 | 59.455 | -1.849 | 26.305 | 1.00 | 31.25 |
| ATOM | 4661 | O | ALA | 608 | 59.791 | -1.054 | 27.198 | 1.00 | 28.90 |
| ATOM | 4662 | N | ARG | 609 | 60.257 | -2.819 | 25.870 | 1.00 | 31.61 |
| ATOM | 4664 | CA | ARG | 609 | 61.608 | -2.979 | 26.393 | 1.00 | 31.99 |
| ATOM | 4665 | CB | ARG | 609 | 62.253 | -4.245 | 25.856 | 1.00 | 34.93 |
| ATOM | 4666 | CG | ARG | 609 | 61.606 | -5.507 | 26.317 | 1.00 | 40.82 |
| ATOM | 4667 | CD | ARG | 609 | 62.633 | -6.606 | 26.397 | 1.00 | 42.68 |
| ATOM | 4668 | NE | ARG | 609 | 63.275 | -6.621 | 27.705 | 1.00 | 43.85 |
| ATOM | 4670 | CZ | ARG | 609 | 64.332 | -7.364 | 28.019 | 1.00 | 44.73 |
| ATOM | 4671 | NH1 | ARG | 609 | 64.889 | -8.162 | 27.108 | 1.00 | 41.40 |
| ATOM | 4674 | NH2 | ARG | 609 | 64.803 | -7.341 | 29.260 | 1.00 | 44.85 |
| ATOM | 4677 | C | ARG | 609 | 62.459 | -1.796 | 25.966 | 1.00 | 33.70 |
| ATOM | 4678 | O | ARG | 609 | 63.130 | -1.174 | 26.793 | 1.00 | 35.94 |
| ATOM | 4679 | N | GLY | 610 | 62.459 | -1.511 | 24.663 | 1.00 | 31.22 |
| ATOM | 4681 | CA | GLY | 610 | 63.232 | -0.391 | 24.157 | 1.00 | 27.21 |
| ATOM | 4682 | C | GLY | 610 | 62.819 | 0.875 | 24.865 | 1.00 | 25.81 |
| ATOM | 4683 | O | GLY | 610 | 63.665 | 1.652 | 25.300 | 1.00 | 26.21 |
| ATOM | 4684 | N | MET | 611 | 61.511 | 1.056 | 25.015 | 1.00 | 27.12 |
| ATOM | 4686 | CA | MET | 611 | 60.969 | 2.222 | 25.695 | 1.00 | 28.82 |
| ATOM | 4687 | CB | MET | 611 | 59.457 | 2.288 | 25.524 | 1.00 | 29.29 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4688 | CG | MET | 611 | 59.004 | 2.706 | 24.135 | 1.00 | 31.07 |
| ATOM | 4689 | SD | MET | 611 | 59.732 | 4.286 | 23.617 | 1.00 | 28.38 |
| ATOM | 4690 | CE | MET | 611 | 59.155 | 5.431 | 24.922 | 1.00 | 28.34 |
| ATOM | 4691 | C | MET | 611 | 61.341 | 2.261 | 27.178 | 1.00 | 30.34 |
| ATOM | 4692 | O | MET | 611 | 61.596 | 3.334 | 27.730 | 1.00 | 31.73 |
| ATOM | 4693 | N | GLU | 612 | 61.347 | 1.109 | 27.837 | 1.00 | 32.72 |
| ATOM | 4695 | CA | GLU | 612 | 61.723 | 1.057 | 29.253 | 1.00 | 35.46 |
| ATOM | 4696 | CB | GLU | 612 | 61.603 | -0.370 | 29.792 | 1.00 | 34.70 |
| ATOM | 4697 | CG | GLU | 612 | 62.029 | -0.516 | 31.237 | 1.00 | 32.31 |
| ATOM | 4698 | CD | GLU | 612 | 62.135 | -1.968 | 31.688 | 1.00 | 33.14 |
| ATOM | 4699 | OE1 | GLU | 612 | 62.546 | -2.834 | 30.883 | 1.00 | 30.79 |
| ATOM | 4700 | OE2 | GLU | 612 | 61.826 | -2.240 | 32.867 | 1.00 | 36.13 |
| ATOM | 4701 | C | GLU | 612 | 63.178 | 1.544 | 29.353 | 1.00 | 36.43 |
| ATOM | 4702 | O | GLU | 612 | 63.534 | 2.319 | 30.261 | 1.00 | 35.38 |
| ATOM | 4703 | N | TYR | 613 | 63.999 | 1.107 | 28.391 | 1.00 | 35.47 |
| ATOM | 4705 | CA | TYR | 613 | 65.403 | 1.507 | 28.334 | 1.00 | 33.16 |
| ATOM | 4706 | CB | TYR | 613 | 66.156 | 0.743 | 27.241 | 1.00 | 31.33 |
| ATOM | 4707 | CG | TYR | 613 | 67.612 | 1.146 | 27.132 | 1.00 | 33.03 |
| ATOM | 4708 | CD1 | TYR | 613 | 68.584 | 0.544 | 27.931 | 1.00 | 36.69 |
| ATOM | 4709 | CE1 | TYR | 613 | 69.930 | 0.927 | 27.851 | 1.00 | 36.82 |
| ATOM | 4710 | CD2 | TYR | 613 | 68.021 | 2.148 | 26.247 | 1.00 | 33.49 |
| ATOM | 4711 | CE2 | TYR | 613 | 69.352 | 2.540 | 26.157 | 1.00 | 34.73 |
| ATOM | 4712 | CZ | TYR | 613 | 70.307 | 1.927 | 26.963 | 1.00 | 37.07 |
| ATOM | 4713 | OH | TYR | 613 | 71.632 | 2.318 | 26.896 | 1.00 | 36.77 |
| ATOM | 4715 | C | TYR | 613 | 65.539 | 3.005 | 28.088 | 1.00 | 31.82 |
| ATOM | 4716 | O | TYR | 613 | 66.256 | 3.682 | 28.814 | 1.00 | 34.76 |
| ATOM | 4717 | N | LEU | 614 | 64.836 | 3.536 | 27.090 | 1.00 | 28.44 |
| ATOM | 4719 | CA | LEU | 614 | 64.931 | 4.956 | 26.793 | 1.00 | 25.67 |
| ATOM | 4720 | CB | LEU | 614 | 64.089 | 5.319 | 25.569 | 1.00 | 24.75 |
| ATOM | 4721 | CG | LEU | 614 | 64.545 | 4.778 | 24.208 | 1.00 | 23.73 |
| ATOM | 4722 | CD1 | LEU | 614 | 63.594 | 5.257 | 23.125 | 1.00 | 20.54 |
| ATOM | 4723 | CD2 | LEU | 614 | 65.983 | 5.213 | 23.894 | 1.00 | 23.21 |
| ATOM | 4724 | C | LEU | 614 | 64.499 | 5.761 | 28.001 | 1.00 | 28.30 |
| ATOM | 4725 | O | LEU | 614 | 65.110 | 6.770 | 28.345 | 1.00 | 27.09 |
| ATOM | 4726 | N | ALA | 615 | 63.470 | 5.272 | 28.683 | 1.00 | 32.73 |
| ATOM | 4728 | CA | ALA | 615 | 62.955 | 5.945 | 29.871 | 1.00 | 34.10 |
| ATOM | 4729 | CB | ALA | 615 | 61.625 | 5.314 | 30.314 | 1.00 | 33.68 |
| ATOM | 4730 | C | ALA | 615 | 63.986 | 5.913 | 31.007 | 1.00 | 33.84 |
| ATOM | 4731 | O | ALA | 615 | 64.112 | 6.885 | 31.753 | 1.00 | 34.95 |
| ATOM | 4732 | N | SER | 616 | 64.722 | 4.809 | 31.134 | 1.00 | 32.69 |
| ATOM | 4734 | CA | SER | 616 | 65.738 | 4.703 | 32.175 | 1.00 | 33.50 |
| ATOM | 4735 | CB | SER | 616 | 66.287 | 3.277 | 32.285 | 1.00 | 28.27 |
| ATOM | 4736 | OG | SER | 616 | 67.076 | 2.935 | 31.165 | 1.00 | 25.54 |
| ATOM | 4738 | C | SER | 616 | 66.870 | 5.678 | 31.865 | 1.00 | 35.43 |
| ATOM | 4739 | O | SER | 616 | 67.637 | 6.061 | 32.755 | 1.00 | 37.32 |
| ATOM | 4740 | N | LYS | 617 | 66.971 | 6.060 | 30.592 | 1.00 | 34.80 |
| ATOM | 4742 | CA | LYS | 617 | 67.975 | 7.010 | 30.143 | 1.00 | 33.01 |
| ATOM | 4743 | CB | LYS | 617 | 68.508 | 6.620 | 28.776 | 1.00 | 33.18 |
| ATOM | 4744 | CG | LYS | 617 | 69.224 | 5.302 | 28.797 | 1.00 | 35.64 |
| ATOM | 4745 | CD | LYS | 617 | 70.423 | 5.380 | 29.710 | 1.00 | 40.31 |
| ATOM | 4746 | CE | LYS | 617 | 71.075 | 4.025 | 29.863 | 1.00 | 43.03 |
| ATOM | 4747 | NZ | LYS | 617 | 72.426 | 4.152 | 30.449 | 1.00 | 45.54 |
| ATOM | 4751 | C | LYS | 617 | 67.360 | 8.397 | 30.102 | 1.00 | 32.87 |
| ATOM | 4752 | O | LYS | 617 | 67.892 | 9.308 | 29.470 | 1.00 | 34.06 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4753 | N | LYS | 618 | 66.221 | 8.542 | 30.772 | 1.00 | 33.53 |
| ATOM | 4755 | CA | LYS | 618 | 65.500 | 9.808 | 30.872 | 1.00 | 33.28 |
| ATOM | 4756 | CB | LYS | 618 | 66.384 | 10.842 | 31.558 | 1.00 | 37.22 |
| ATOM | 4757 | CG | LYS | 618 | 66.968 | 10.367 | 32.869 | 1.00 | 43.11 |
| ATOM | 4758 | CD | LYS | 618 | 65.927 | 10.278 | 33.957 | 1.00 | 49.82 |
| ATOM | 4759 | CE | LYS | 618 | 66.520 | 9.636 | 35.199 | 1.00 | 55.20 |
| ATOM | 4760 | NZ | LYS | 618 | 65.669 | 9.853 | 36.415 | 1.00 | 61.31 |
| ATOM | 4764 | C | LYS | 618 | 65.012 | 10.359 | 29.542 | 1.00 | 31.57 |
| ATOM | 4765 | O | LYS | 618 | 64.651 | 11.530 | 29.455 | 1.00 | 31.10 |
| ATOM | 4766 | N | CYS | 619 | 64.953 | 9.506 | 28.524 | 1.00 | 31.04 |
| ATOM | 4768 | CA | CYS | 619 | 64.519 | 9.922 | 27.196 | 1.00 | 29.21 |
| ATOM | 4769 | CB | CYS | 619 | 65.213 | 9.065 | 26.125 | 1.00 | 28.55 |
| ATOM | 4770 | SG | CYS | 619 | 64.782 | 9.400 | 24.392 | 1.00 | 26.31 |
| ATOM | 4771 | C | CYS | 619 | 62.999 | 9.849 | 27.051 | 1.00 | 30.91 |
| ATOM | 4772 | O | CYS | 619 | 62.376 | 8.827 | 27.364 | 1.00 | 31.18 |
| ATOM | 4773 | N | ILE | 620 | 62.411 | 10.967 | 26.632 | 1.00 | 29.48 |
| ATOM | 4775 | CA | ILE | 620 | 60.981 | 11.073 | 26.416 | 1.00 | 29.34 |
| ATOM | 4776 | CB | ILE | 620 | 60.402 | 12.344 | 27.060 | 1.00 | 28.12 |
| ATOM | 4777 | CG2 | ILE | 620 | 58.944 | 12.535 | 26.645 | 1.00 | 28.76 |
| ATOM | 4778 | CG1 | ILE | 620 | 60.521 | 12.267 | 28.581 | 1.00 | 28.36 |
| ATOM | 4779 | CD1 | ILE | 620 | 60.062 | 13.522 | 29.270 | 1.00 | 25.55 |
| ATOM | 4780 | C | ILE | 620 | 60.852 | 11.188 | 24.908 | 1.00 | 30.97 |
| ATOM | 4781 | O | ILE | 620 | 61.254 | 12.193 | 24.336 | 1.00 | 33.88 |
| ATOM | 4782 | N | HIS | 621 | 60.307 | 10.147 | 24.284 | 1.00 | 31.55 |
| ATOM | 4784 | CA | HIS | 621 | 60.148 | 10.080 | 22.831 | 1.00 | 31.85 |
| ATOM | 4785 | CB | HIS | 621 | 59.721 | 8.668 | 22.425 | 1.00 | 28.27 |
| ATOM | 4786 | CG | HIS | 621 | 59.913 | 8.373 | 20.979 | 1.00 | 24.68 |
| ATOM | 4787 | CD2 | HIS | 621 | 60.608 | 7.383 | 20.356 | 1.00 | 24.39 |
| ATOM | 4788 | ND1 | HIS | 621 | 59.354 | 9.130 | 19.973 | 1.00 | 25.87 |
| ATOM | 4790 | CE1 | HIS | 621 | 59.691 | 8.623 | 18.798 | 1.00 | 27.65 |
| ATOM | 4791 | NE2 | HIS | 621 | 60.444 | 7.571 | 19.007 | 1.00 | 25.80 |
| ATOM | 4793 | C | HIS | 621 | 59.187 | 11.096 | 22.224 | 1.00 | 34.38 |
| ATOM | 4794 | O | HIS | 621 | 59.387 | 11.539 | 21.104 | 1.00 | 38.74 |
| ATOM | 4795 | N | ARG | 622 | 58.080 | 11.374 | 22.898 | 1.00 | 37.17 |
| ATOM | 4797 | CA | ARG | 622 | 57.093 | 12.346 | 22.425 | 1.00 | 37.27 |
| ATOM | 4798 | CB | ARG | 622 | 57.718 | 13.746 | 22.298 | 1.00 | 38.63 |
| ATOM | 4799 | CG | ARG | 622 | 58.261 | 14.271 | 23.601 | 1.00 | 40.47 |
| ATOM | 4800 | CD | ARG | 622 | 58.661 | 15.739 | 23.530 | 1.00 | 44.76 |
| ATOM | 4801 | NE | ARG | 622 | 59.129 | 16.174 | 24.842 | 1.00 | 52.09 |
| ATOM | 4803 | CZ | ARG | 622 | 60.299 | 15.821 | 25.375 | 1.00 | 56.86 |
| ATOM | 4804 | NH1 | ARG | 622 | 61.132 | 15.041 | 24.699 | 1.00 | 61.20 |
| ATOM | 4807 | NH2 | ARG | 622 | 60.606 | 16.167 | 26.624 | 1.00 | 58.19 |
| ATOM | 4810 | C | ARG | 622 | 56.324 | 11.994 | 21.151 | 1.00 | 37.23 |
| ATOM | 4811 | O | ARG | 622 | 55.300 | 12.614 | 20.867 | 1.00 | 38.45 |
| ATOM | 4812 | N | ASP | 623 | 56.805 | 11.035 | 20.364 | 1.00 | 36.55 |
| ATOM | 4814 | CA | ASP | 623 | 56.075 | 10.652 | 19.160 | 1.00 | 36.52 |
| ATOM | 4815 | CB | ASP | 623 | 56.581 | 11.403 | 17.910 | 1.00 | 39.68 |
| ATOM | 4816 | CG | ASP | 623 | 55.635 | 11.247 | 16.687 | 1.00 | 48.75 |
| ATOM | 4817 | OD1 | ASP | 623 | 56.077 | 11.491 | 15.538 | 1.00 | 49.98 |
| ATOM | 4818 | OD2 | ASP | 623 | 54.445 | 10.879 | 16.872 | 1.00 | 49.65 |
| ATOM | 4819 | C | ASP | 623 | 56.126 | 9.143 | 18.967 | 1.00 | 33.37 |
| ATOM | 4820 | O | ASP | 623 | 56.325 | 8.650 | 17.864 | 1.00 | 31.77 |
| ATOM | 4821 | N | LEU | 624 | 55.999 | 8.404 | 20.059 | 1.00 | 30.45 |
| ATOM | 4823 | CA | LEU | 624 | 56.014 | 6.954 | 19.950 | 1.00 | 30.77 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4824 | CB | LEU | 624 | 55.983 | 6.307 | 21.342 | 1.00 | 27.43 |
| ATOM | 4825 | CG | LEU | 624 | 55.949 | 4.778 | 21.441 | 1.00 | 28.69 |
| ATOM | 4826 | CD1 | LEU | 624 | 57.139 | 4.132 | 20.731 | 1.00 | 24.75 |
| ATOM | 4827 | CD2 | LEU | 624 | 55.927 | 4.389 | 22.894 | 1.00 | 27.39 |
| ATOM | 4828 | C | LEU | 624 | 54.803 | 6.532 | 19.109 | 1.00 | 31.22 |
| ATOM | 4829 | O | LEU | 624 | 53.680 | 6.952 | 19.380 | 1.00 | 33.44 |
| ATOM | 4830 | N | ALA | 625 | 55.053 | 5.763 | 18.054 | 1.00 | 28.85 |
| ATOM | 4832 | CA | ALA | 625 | 54.009 | 5.286 | 17.159 | 1.00 | 26.93 |
| ATOM | 4833 | CB | ALA | 625 | 53.559 | 6.400 | 16.227 | 1.00 | 25.03 |
| ATOM | 4834 | C | ALA | 625 | 54.642 | 4.162 | 16.356 | 1.00 | 28.44 |
| ATOM | 4835 | O | ALA | 625 | 55.863 | 4.065 | 16.317 | 1.00 | 31.32 |
| ATOM | 4836 | N | ALA | 626 | 53.828 | 3.329 | 15.705 | 1.00 | 29.14 |
| ATOM | 4838 | CA | ALA | 626 | 54.344 | 2.205 | 14.905 | 1.00 | 28.42 |
| ATOM | 4839 | CB | ALA | 626 | 53.192 | 1.357 | 14.353 | 1.00 | 27.37 |
| ATOM | 4840 | C | ALA | 626 | 55.231 | 2.698 | 13.771 | 1.00 | 26.38 |
| ATOM | 4841 | O | ALA | 626 | 56.195 | 2.041 | 13.395 | 1.00 | 26.12 |
| ATOM | 4842 | N | ARG | 627 | 54.890 | 3.861 | 13.230 | 1.00 | 27.16 |
| ATOM | 4844 | CA | ARG | 627 | 55.669 | 4.474 | 12.158 | 1.00 | 28.44 |
| ATOM | 4845 | CB | ARG | 627 | 55.022 | 5.794 | 11.733 | 1.00 | 28.19 |
| ATOM | 4846 | CG | ARG | 627 | 54.889 | 6.793 | 12.867 | 1.00 | 30.34 |
| ATOM | 4847 | CD | ARG | 627 | 54.456 | 8.155 | 12.361 | 1.00 | 34.08 |
| ATOM | 4848 | NE | ARG | 627 | 54.081 | 9.024 | 13.471 | 1.00 | 35.58 |
| ATOM | 4850 | CZ | ARG | 627 | 52.849 | 9.123 | 13.950 | 1.00 | 35.55 |
| ATOM | 4851 | NH1 | ARG | 627 | 51.860 | 8.422 | 13.420 | 1.00 | 35.67 |
| ATOM | 4854 | NH2 | ARG | 627 | 52.618 | 9.898 | 14.993 | 1.00 | 40.81 |
| ATOM | 4857 | C | ARG | 627 | 57.108 | 4.733 | 12.630 | 1.00 | 28.06 |
| ATOM | 4858 | O | ARG | 627 | 58.044 | 4.737 | 11.825 | 1.00 | 29.80 |
| ATOM | 4859 | N | ASN | 628 | 57.272 | 4.935 | 13.940 | 1.00 | 28.50 |
| ATOM | 4861 | CA | ASN | 628 | 58.582 | 5.195 | 14.544 | 1.00 | 26.14 |
| ATOM | 4862 | CB | ASN | 628 | 58.494 | 6.340 | 15.551 | 1.00 | 23.55 |
| ATOM | 4863 | CG | ASN | 628 | 58.319 | 7.681 | 14.874 | 1.00 | 27.48 |
| ATOM | 4864 | OD1 | ASN | 628 | 58.874 | 7.919 | 13.800 | 1.00 | 34.12 |
| ATOM | 4865 | ND2 | ASN | 628 | 57.543 | 8.556 | 15.479 | 1.00 | 23.21 |
| ATOM | 4868 | C | ASN | 628 | 59.263 | 3.965 | 15.153 | 1.00 | 26.76 |
| ATOM | 4869 | O | ASN | 628 | 60.202 | 4.078 | 15.948 | 1.00 | 26.90 |
| ATOM | 4870 | N | VAL | 629 | 58.774 | 2.794 | 14.767 | 1.00 | 27.02 |
| ATOM | 4872 | CA | VAL | 629 | 59.344 | 1.523 | 15.186 | 1.00 | 27.81 |
| ATOM | 4873 | CB | VAL | 629 | 58.298 | 0.622 | 15.864 | 1.00 | 26.83 |
| ATOM | 4874 | CG1 | VAL | 629 | 58.876 | -0.766 | 16.115 | 1.00 | 20.74 |
| ATOM | 4875 | CG2 | VAL | 629 | 57.836 | 1.259 | 17.165 | 1.00 | 22.49 |
| ATOM | 4876 | C | VAL | 629 | 59.781 | 0.895 | 13.861 | 1.00 | 28.61 |
| ATOM | 4877 | O | VAL | 629 | 58.983 | 0.809 | 12.924 | 1.00 | 28.76 |
| ATOM | 4878 | N | LEU | 630 | 61.059 | 0.557 | 13.746 | 1.00 | 30.35 |
| ATOM | 4880 | CA | LEU | 630 | 61.576 | -0.033 | 12.514 | 1.00 | 32.42 |
| ATOM | 4881 | CB | LEU | 630 | 62.824 | 0.725 | 12.040 | 1.00 | 32.28 |
| ATOM | 4882 | CG | LEU | 630 | 62.697 | 2.249 | 11.880 | 1.00 | 27.75 |
| ATOM | 4883 | CD1 | LEU | 630 | 64.019 | 2.860 | 11.469 | 1.00 | 24.71 |
| ATOM | 4884 | CD2 | LEU | 630 | 61.611 | 2.582 | 10.872 | 1.00 | 27.70 |
| ATOM | 4885 | C | LEU | 630 | 61.895 | -1.488 | 12.799 | 1.00 | 32.89 |
| ATOM | 4886 | O | LEU | 630 | 62.167 | -1.838 | 13.943 | 1.00 | 32.32 |
| ATOM | 4887 | N | VAL | 631 | 61.831 | -2.336 | 11.774 | 1.00 | 34.81 |
| ATOM | 4889 | CA | VAL | 631 | 62.087 | -3.772 | 11.943 | 1.00 | 33.87 |
| ATOM | 4890 | CB | VAL | 631 | 60.818 | -4.616 | 11.597 | 1.00 | 31.60 |
| ATOM | 4891 | CG1 | VAL | 631 | 60.929 | -6.004 | 12.197 | 1.00 | 30.84 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4892 | CG2 | VAL | 631 | 59.545 | -3.916 | 12.089 | 1.00 | 25.53 |
| ATOM | 4893 | C | VAL | 631 | 63.286 | -4.256 | 11.109 | 1.00 | 34.95 |
| ATOM | 4894 | O | VAL | 631 | 63.365 | -4.009 | 9.892 | 1.00 | 37.01 |
| ATOM | 4895 | N | THR | 632 | 64.215 | -4.942 | 11.770 | 1.00 | 35.08 |
| ATOM | 4897 | CA | THR | 632 | 65.418 | -5.444 | 11.104 | 1.00 | 35.96 |
| ATOM | 4898 | CB | THR | 632 | 66.541 | -5.711 | 12.116 | 1.00 | 34.29 |
| ATOM | 4899 | OG1 | THR | 632 | 66.187 | -6.818 | 12.953 | 1.00 | 32.35 |
| ATOM | 4901 | CG2 | THR | 632 | 66.750 | -4.488 | 12.985 | 1.00 | 33.42 |
| ATOM | 4902 | C | THR | 632 | 65.162 | -6.712 | 10.300 | 1.00 | 39.32 |
| ATOM | 4903 | O | THR | 632 | 64.078 | -7.302 | 10.382 | 1.00 | 41.24 |
| ATOM | 4904 | N | GLU | 633 | 66.153 | -7.123 | 9.511 | 1.00 | 42.32 |
| ATOM | 4906 | CA | GLU | 633 | 66.030 | -8.335 | 8.703 | 1.00 | 44.34 |
| ATOM | 4907 | CB | GLU | 633 | 67.314 | -8.609 | 7.912 | 1.00 | 46.06 |
| ATOM | 4908 | CG | GLU | 633 | 67.205 | -9.767 | 6.898 | 1.00 | 49.87 |
| ATOM | 4909 | CD | GLU | 633 | 66.380 | -9.445 | 5.629 | 1.00 | 53.04 |
| ATOM | 4910 | OE1 | GLU | 633 | 65.637 | -8.430 | 5.570 | 1.00 | 51.31 |
| ATOM | 4911 | OE2 | GLU | 633 | 66.479 | -10.226 | 4.667 | 1.00 | 55.48 |
| ATOM | 4912 | C | GLU | 633 | 65.708 | -9.526 | 9.600 | 1.00 | 44.58 |
| ATOM | 4913 | O | GLU | 633 | 64.974 | -10.423 | 9.207 | 1.00 | 46.56 |
| ATOM | 4914 | N | ASP | 634 | 66.201 | -9.493 | 10.833 | 1.00 | 44.12 |
| ATOM | 4916 | CA | ASP | 634 | 65.961 | -10.583 | 11.759 | 1.00 | 44.23 |
| ATOM | 4917 | CB | ASP | 634 | 67.221 | -10.867 | 12.580 | 1.00 | 50.17 |
| ATOM | 4918 | CG | ASP | 634 | 68.443 | -11.181 | 11.697 | 1.00 | 56.79 |
| ATOM | 4919 | OD1 | ASP | 634 | 68.363 | -12.113 | 10.857 | 1.00 | 59.62 |
| ATOM | 4920 | OD2 | ASP | 634 | 69.482 | -10.490 | 11.837 | 1.00 | 58.62 |
| ATOM | 4921 | C | ASP | 634 | 64.756 | -10.331 | 12.644 | 1.00 | 43.26 |
| ATOM | 4922 | O | ASP | 634 | 64.652 | -10.879 | 13.733 | 1.00 | 43.58 |
| ATOM | 4923 | N | ASN | 635 | 63.858 | -9.475 | 12.166 | 1.00 | 43.97 |
| ATOM | 4925 | CA | ASN | 635 | 62.612 | -9.126 | 12.847 | 1.00 | 43.66 |
| ATOM | 4926 | CB | ASN | 635 | 61.698 | -10.355 | 12.930 | 1.00 | 46.94 |
| ATOM | 4927 | CG | ASN | 635 | 61.413 | -10.958 | 11.572 | 1.00 | 48.19 |
| ATOM | 4928 | OD1 | ASN | 635 | 60.831 | -10.314 | 10.702 | 1.00 | 51.42 |
| ATOM | 4929 | ND2 | ASN | 635 | 61.832 | -12.198 | 11.380 | 1.00 | 49.44 |
| ATOM | 4932 | C | ASN | 635 | 62.694 | -8.463 | 14.216 | 1.00 | 43.03 |
| ATOM | 4933 | O | ASN | 635 | 61.774 | -8.596 | 15.031 | 1.00 | 43.03 |
| ATOM | 4934 | N | VAL | 636 | 63.763 | -7.712 | 14.467 | 1.00 | 42.69 |
| ATOM | 4936 | CA | VAL | 636 | 63.915 | -7.034 | 15.756 | 1.00 | 38.30 |
| ATOM | 4937 | CB | VAL | 636 | 65.406 | -6.861 | 16.134 | 1.00 | 37.92 |
| ATOM | 4938 | CG1 | VAL | 636 | 65.555 | -6.040 | 17.421 | 1.00 | 37.14 |
| ATOM | 4939 | CG2 | VAL | 636 | 66.052 | -8.226 | 16.306 | 1.00 | 37.55 |
| ATOM | 4940 | C | VAL | 636 | 63.251 | -5.673 | 15.688 | 1.00 | 35.75 |
| ATOM | 4941 | O | VAL | 636 | 63.486 | -4.926 | 14.746 | 1.00 | 36.28 |
| ATOM | 4942 | N | MET | 637 | 62.355 | -5.396 | 16.628 | 1.00 | 34.73 |
| ATOM | 4944 | CA | MET | 637 | 61.672 | -4.103 | 16.680 | 1.00 | 33.22 |
| ATOM | 4945 | CB | MET | 637 | 60.456 | -4.152 | 17.608 | 1.00 | 34.83 |
| ATOM | 4946 | CG | MET | 637 | 59.364 | -5.148 | 17.231 | 1.00 | 34.41 |
| ATOM | 4947 | SD | MET | 637 | 58.661 | -4.926 | 15.589 | 1.00 | 33.19 |
| ATOM | 4948 | CE | MET | 637 | 58.869 | -6.584 | 14.913 | 1.00 | 29.73 |
| ATOM | 4949 | C | MET | 637 | 62.677 | -3.107 | 17.250 | 1.00 | 33.75 |
| ATOM | 4950 | O | MET | 637 | 63.281 | -3.357 | 18.308 | 1.00 | 31.79 |
| ATOM | 4951 | N | LYS | 638 | 62.839 | -1.980 | 16.558 | 1.00 | 31.83 |
| ATOM | 4953 | CA | LYS | 638 | 63.774 | -0.939 | 16.965 | 1.00 | 28.17 |
| ATOM | 4954 | CB | LYS | 638 | 64.986 | -0.930 | 16.038 | 1.00 | 24.98 |
| ATOM | 4955 | CG | LYS | 638 | 66.006 | -1.967 | 16.400 | 1.00 | 23.17 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4956 | CD | LYS | 638 | 67.193 | -1.916 | 15.470 | 1.00 | 25.04 |
| ATOM | 4957 | CE | LYS | 638 | 68.212 | -2.969 | 15.847 | 1.00 | 24.79 |
| ATOM | 4958 | NZ | LYS | 638 | 68.747 | -2.765 | 17.220 | 1.00 | 24.91 |
| ATOM | 4962 | C | LYS | 638 | 63.165 | 0.445 | 16.986 | 1.00 | 26.04 |
| ATOM | 4963 | O | LYS | 638 | 62.803 | 0.958 | 15.936 | 1.00 | 24.44 |
| ATOM | 4964 | N | ILE | 639 | 63.052 | 1.031 | 18.181 | 1.00 | 25.14 |
| ATOM | 4966 | CA | ILE | 639 | 62.508 | 2.376 | 18.351 | 1.00 | 25.68 |
| ATOM | 4967 | CB | ILE | 639 | 62.589 | 2.863 | 19.839 | 1.00 | 27.40 |
| ATOM | 4968 | CG2 | ILE | 639 | 61.875 | 4.189 | 19.984 | 1.00 | 18.94 |
| ATOM | 4969 | CG1 | ILE | 639 | 62.019 | 1.827 | 20.826 | 1.00 | 26.05 |
| ATOM | 4970 | CD1 | ILE | 639 | 60.517 | 1.667 | 20.792 | 1.00 | 25.07 |
| ATOM | 4971 | C | ILE | 639 | 63.387 | 3.338 | 17.543 | 1.00 | 25.82 |
| ATOM | 4972 | O | ILE | 639 | 64.619 | 3.283 | 17.642 | 1.00 | 25.76 |
| ATOM | 4973 | N | ALA | 640 | 62.758 | 4.231 | 16.783 | 1.00 | 25.92 |
| ATOM | 4975 | CA | ALA | 640 | 63.477 | 5.218 | 15.976 | 1.00 | 26.12 |
| ATOM | 4976 | CB | ALA | 640 | 63.222 | 4.964 | 14.506 | 1.00 | 26.54 |
| ATOM | 4977 | C | ALA | 640 | 63.042 | 6.643 | 16.344 | 1.00 | 26.33 |
| ATOM | 4978 | O | ALA | 640 | 61.996 | 6.828 | 16.974 | 1.00 | 26.20 |
| ATOM | 4979 | N | ASP | 641 | 63.863 | 7.637 | 15.993 | 1.00 | 26.59 |
| ATOM | 4981 | CA | ASP | 641 | 63.545 | 9.052 | 16.245 | 1.00 | 28.09 |
| ATOM | 4982 | CB | ASP | 641 | 62.217 | 9.443 | 15.593 | 1.00 | 31.43 |
| ATOM | 4983 | CG | ASP | 641 | 62.346 | 9.762 | 14.107 | 1.00 | 36.81 |
| ATOM | 4984 | OD1 | ASP | 641 | 63.409 | 9.478 | 13.500 | 1.00 | 40.24 |
| ATOM | 4985 | OD2 | ASP | 641 | 61.356 | 10.299 | 13.548 | 1.00 | 40.49 |
| ATOM | 4986 | C | ASP | 641 | 63.455 | 9.442 | 17.700 | 1.00 | 28.40 |
| ATOM | 4987 | O | ASP | 641 | 62.825 | 10.446 | 18.041 | 1.00 | 29.30 |
| ATOM | 4988 | N | PHE | 642 | 64.080 | 8.658 | 18.564 | 1.00 | 30.27 |
| ATOM | 4990 | CA | PHE | 642 | 64.044 | 8.943 | 19.992 | 1.00 | 30.97 |
| ATOM | 4991 | CB | PHE | 642 | 64.327 | 7.664 | 20.787 | 1.00 | 24.64 |
| ATOM | 4992 | CG | PHE | 642 | 65.673 | 7.063 | 20.505 | 1.00 | 20.96 |
| ATOM | 4993 | CD1 | PHE | 642 | 66.812 | 7.539 | 21.163 | 1.00 | 16.89 |
| ATOM | 4994 | CD2 | PHE | 642 | 65.806 | 6.026 | 19.576 | 1.00 | 16.23 |
| ATOM | 4995 | CE1 | PHE | 642 | 68.072 | 6.990 | 20.900 | 1.00 | 18.35 |
| ATOM | 4996 | CE2 | PHE | 642 | 67.051 | 5.471 | 19.305 | 1.00 | 18.76 |
| ATOM | 4997 | CZ | PHE | 642 | 68.195 | 5.954 | 19.970 | 1.00 | 17.91 |
| ATOM | 4998 | C | PHE | 642 | 65.024 | 10.045 | 20.414 | 1.00 | 34.53 |
| ATOM | 4999 | O | PHE | 642 | 64.990 | 10.503 | 21.563 | 1.00 | 35.23 |
| ATOM | 5000 | N | GLY | 643 | 65.910 | 10.433 | 19.500 | 1.00 | 36.40 |
| ATOM | 5002 | CA | GLY | 643 | 66.888 | 11.455 | 19.799 | 1.00 | 38.28 |
| ATOM | 5003 | C | GLY | 643 | 66.634 | 12.768 | 19.093 | 1.00 | 41.44 |
| ATOM | 5004 | O | GLY | 643 | 67.482 | 13.652 | 19.132 | 1.00 | 44.10 |
| ATOM | 5005 | N | LEU | 644 | 65.461 | 12.921 | 18.484 | 1.00 | 45.44 |
| ATOM | 5007 | CA | LEU | 644 | 65.131 | 14.144 | 17.748 | 1.00 | 49.14 |
| ATOM | 5008 | CB | LEU | 644 | 63.832 | 13.975 | 16.969 | 1.00 | 46.26 |
| ATOM | 5009 | CG | LEU | 644 | 63.823 | 12.967 | 15.836 | 1.00 | 42.90 |
| ATOM | 5010 | CD1 | LEU | 644 | 62.527 | 13.134 | 15.070 | 1.00 | 42.68 |
| ATOM | 5011 | CD2 | LEU | 644 | 65.004 | 13.228 | 14.934 | 1.00 | 45.15 |
| ATOM | 5012 | C | LEU | 644 | 65.027 | 15.396 | 18.605 | 1.00 | 53.90 |
| ATOM | 5013 | O | LEU | 644 | 64.488 | 15.356 | 19.715 | 1.00 | 56.54 |
| ATOM | 5014 | N | ALA | 645 | 65.534 | 16.505 | 18.068 | 1.00 | 57.59 |
| ATOM | 5016 | CA | ALA | 645 | 65.505 | 17.794 | 18.759 | 1.00 | 60.15 |
| ATOM | 5017 | CB | ALA | 645 | 66.539 | 18.741 | 18.156 | 1.00 | 59.55 |
| ATOM | 5018 | C | ALA | 645 | 64.112 | 18.407 | 18.667 | 1.00 | 61.90 |
| ATOM | 5019 | O | ALA | 645 | 63.393 | 18.500 | 19.663 | 1.00 | 63.83 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5020 | N | ASP | 652 | 52.090 | 22.191 | 14.865 | 1.00 | 89.91 |
| ATOM | 5022 | CA | ASP | 652 | 50.913 | 22.199 | 14.007 | 1.00 | 89.75 |
| ATOM | 5023 | CB | ASP | 652 | 51.314 | 22.428 | 12.537 | 1.00 | 88.08 |
| ATOM | 5024 | CG | ASP | 652 | 50.109 | 22.557 | 11.607 | 1.00 | 87.09 |
| ATOM | 5025 | OD1 | ASP | 652 | 49.028 | 22.996 | 12.052 | 1.00 | 86.85 |
| ATOM | 5026 | OD2 | ASP | 652 | 50.252 | 22.222 | 10.411 | 1.00 | 86.69 |
| ATOM | 5027 | C | ASP | 652 | 50.145 | 20.890 | 14.156 | 1.00 | 89.98 |
| ATOM | 5028 | O | ASP | 652 | 50.434 | 19.899 | 13.483 | 1.00 | 90.19 |
| ATOM | 5029 | N | TYR | 653 | 49.145 | 20.905 | 15.027 | 1.00 | 90.26 |
| ATOM | 5031 | CA | TYR | 653 | 48.318 | 19.730 | 15.277 | 1.00 | 90.78 |
| ATOM | 5032 | CB | TYR | 653 | 47.272 | 20.048 | 16.344 | 1.00 | 91.65 |
| ATOM | 5033 | CG | TYR | 653 | 47.804 | 20.185 | 17.755 | 1.00 | 93.43 |
| ATOM | 5034 | CD1 | TYR | 653 | 47.017 | 20.757 | 18.752 | 1.00 | 94.60 |
| ATOM | 5035 | CE1 | TYR | 653 | 47.477 | 20.885 | 20.058 | 1.00 | 95.35 |
| ATOM | 5036 | CD2 | TYR | 653 | 49.083 | 19.738 | 18.101 | 1.00 | 93.46 |
| ATOM | 5037 | CE2 | TYR | 653 | 49.558 | 19.860 | 19.406 | 1.00 | 94.36 |
| ATOM | 5038 | CZ | TYR | 653 | 48.748 | 20.435 | 20.378 | 1.00 | 95.26 |
| ATOM | 5039 | OH | TYR | 653 | 49.220 | 20.554 | 21.669 | 1.00 | 95.00 |
| ATOM | 5041 | C | TYR | 653 | 47.602 | 19.231 | 14.021 | 1.00 | 90.47 |
| ATOM | 5042 | O | TYR | 653 | 47.045 | 18.131 | 14.012 | 1.00 | 91.33 |
| ATOM | 5043 | N | TYR | 654 | 47.632 | 20.031 | 12.962 | 1.00 | 89.21 |
| ATOM | 5045 | CA | TYR | 654 | 46.954 | 19.673 | 11.727 | 1.00 | 89.09 |
| ATOM | 5046 | CB | TYR | 654 | 46.205 | 20.893 | 11.188 | 1.00 | 88.23 |
| ATOM | 5047 | CG | TYR | 654 | 45.275 | 21.499 | 12.209 | 1.00 | 87.65 |
| ATOM | 5048 | CD1 | TYR | 654 | 45.776 | 22.140 | 13.343 | 1.00 | 86.76 |
| ATOM | 5049 | CE1 | TYR | 654 | 44.929 | 22.655 | 14.312 | 1.00 | 87.17 |
| ATOM | 5050 | CD2 | TYR | 654 | 43.895 | 21.396 | 12.067 | 1.00 | 88.61 |
| ATOM | 5051 | CE2 | TYR | 654 | 43.032 | 21.912 | 13.033 | 1.00 | 89.32 |
| ATOM | 5052 | CZ | TYR | 654 | 43.557 | 22.538 | 14.153 | 1.00 | 88.66 |
| ATOM | 5053 | OH | TYR | 654 | 42.710 | 23.034 | 15.117 | 1.00 | 89.39 |
| ATOM | 5055 | C | TYR | 654 | 47.857 | 19.080 | 10.651 | 1.00 | 89.49 |
| ATOM | 5056 | O | TYR | 654 | 47.396 | 18.772 | 9.552 | 1.00 | 88.37 |
| ATOM | 5057 | N | LYS | 655 | 49.139 | 18.919 | 10.959 | 1.00 | 90.80 |
| ATOM | 5059 | CA | LYS | 655 | 50.056 | 18.356 | 9.982 | 1.00 | 93.18 |
| ATOM | 5060 | CB | LYS | 655 | 51.508 | 18.713 | 10.311 | 1.00 | 95.66 |
| ATOM | 5061 | CG | LYS | 655 | 52.504 | 18.133 | 9.315 | 1.00 | 99.82 |
| ATOM | 5062 | CD | LYS | 655 | 53.932 | 18.585 | 9.562 | 1.00103.58 | |
| ATOM | 5063 | CE | LYS | 655 | 54.898 | 17.833 | 8.637 | 1.00106.15 | |
| ATOM | 5064 | NZ | LYS | 655 | 56.325 | 18.246 | 8.821 | 1.00108.43 | |
| ATOM | 5068 | C | LYS | 655 | 49.884 | 16.847 | 9.935 | 1.00 | 93.56 |
| ATOM | 5069 | O | LYS | 655 | 49.904 | 16.182 | 10.972 | 1.00 | 93.72 |
| ATOM | 5070 | N | LYS | 656 | 49.670 | 16.320 | 8.735 | 1.00 | 94.19 |
| ATOM | 5072 | CA | LYS | 656 | 49.500 | 14.886 | 8.545 | 1.00 | 94.84 |
| ATOM | 5073 | CB | LYS | 656 | 48.628 | 14.620 | 7.320 | 1.00 | 94.64 |
| ATOM | 5074 | CG | LYS | 656 | 47.155 | 14.874 | 7.542 | 1.00 | 95.54 |
| ATOM | 5075 | CD | LYS | 656 | 46.402 | 14.709 | 6.241 | 1.00 | 99.56 |
| ATOM | 5076 | CE | LYS | 656 | 44.926 | 14.449 | 6.473 | 1.00101.77 | |
| ATOM | 5077 | NZ | LYS | 656 | 44.202 | 14.327 | 5.173 | 1.00103.77 | |
| ATOM | 5081 | C | LYS | 656 | 50.859 | 14.225 | 8.368 | 1.00 | 95.18 |
| ATOM | 5082 | O | LYS | 656 | 51.823 | 14.878 | 7.956 | 1.00 | 95.74 |
| ATOM | 5083 | N | GLY | 660 | 48.651 | 9.665 | 5.782 | 1.00 | 58.76 |
| ATOM | 5085 | CA | GLY | 660 | 47.932 | 10.910 | 6.012 | 1.00 | 56.04 |
| ATOM | 5086 | C | GLY | 660 | 47.241 | 10.937 | 7.364 | 1.00 | 53.90 |
| ATOM | 5087 | O | GLY | 660 | 46.183 | 11.552 | 7.525 | 1.00 | 53.92 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5088 | N | ARG | 661 | 47.838 | 10.243 | 8.328 | 1.00 | 51.87 |
| ATOM | 5090 | CA | ARG | 661 | 47.297 | 10.177 | 9.679 | 1.00 | 48.23 |
| ATOM | 5091 | CB | ARG | 661 | 47.755 | 8.891 | 10.377 | 1.00 | 49.74 |
| ATOM | 5092 | CG | ARG | 661 | 47.506 | 7.620 | 9.566 | 1.00 | 47.59 |
| ATOM | 5093 | CD | ARG | 661 | 47.561 | 6.390 | 10.446 | 1.00 | 51.85 |
| ATOM | 5094 | NE | ARG | 661 | 47.584 | 5.155 | 9.663 | 1.00 | 52.94 |
| ATOM | 5096 | CZ | ARG | 661 | 48.035 | 3.988 | 10.117 | 1.00 | 52.19 |
| ATOM | 5097 | NH1 | ARG | 661 | 48.503 | 3.884 | 11.356 | 1.00 | 52.10 |
| ATOM | 5100 | NH2 | ARG | 661 | 48.036 | 2.926 | 9.327 | 1.00 | 54.43 |
| ATOM | 5103 | C | ARG | 661 | 47.722 | 11.401 | 10.483 | 1.00 | 43.67 |
| ATOM | 5104 | O | ARG | 661 | 48.658 | 12.103 | 10.104 | 1.00 | 41.45 |
| ATOM | 5105 | N | LEU | 662 | 47.019 | 11.656 | 11.579 | 1.00 | 40.27 |
| ATOM | 5107 | CA | LEU | 662 | 47.310 | 12.799 | 12.437 | 1.00 | 37.15 |
| ATOM | 5108 | CB | LEU | 662 | 46.021 | 13.533 | 12.783 | 1.00 | 37.39 |
| ATOM | 5109 | CG | LEU | 662 | 45.301 | 14.149 | 11.588 | 1.00 | 37.67 |
| ATOM | 5110 | CD1 | LEU | 662 | 43.852 | 14.428 | 11.937 | 1.00 | 35.38 |
| ATOM | 5111 | CD2 | LEU | 662 | 46.041 | 15.407 | 11.163 | 1.00 | 39.79 |
| ATOM | 5112 | C | LEU | 662 | 47.973 | 12.330 | 13.716 | 1.00 | 34.68 |
| ATOM | 5113 | O | LEU | 662 | 47.327 | 11.718 | 14.568 | 1.00 | 33.33 |
| ATOM | 5114 | N | PRO | 663 | 49.260 | 12.655 | 13.892 | 1.00 | 34.11 |
| ATOM | 5115 | CD | PRO | 663 | 50.086 | 13.389 | 12.924 | 1.00 | 33.67 |
| ATOM | 5116 | CA | PRO | 663 | 50.052 | 12.281 | 15.068 | 1.00 | 33.55 |
| ATOM | 5117 | CB | PRO | 663 | 51.367 | 13.003 | 14.833 | 1.00 | 32.99 |
| ATOM | 5118 | CG | PRO | 663 | 51.479 | 12.966 | 13.328 | 1.00 | 36.09 |
| ATOM | 5119 | C | PRO | 663 | 49.412 | 12.665 | 16.399 | 1.00 | 33.55 |
| ATOM | 5120 | O | PRO | 663 | 49.683 | 12.036 | 17.426 | 1.00 | 34.11 |
| ATOM | 5121 | N | VAL | 664 | 48.566 | 13.697 | 16.387 | 1.00 | 32.63 |
| ATOM | 5123 | CA | VAL | 664 | 47.874 | 14.092 | 17.613 | 1.00 | 32.24 |
| ATOM | 5124 | CB | VAL | 664 | 46.953 | 15.327 | 17.396 | 1.00 | 33.24 |
| ATOM | 5125 | CG1 | VAL | 664 | 47.779 | 16.583 | 17.252 | 1.00 | 35.01 |
| ATOM | 5126 | CG2 | VAL | 664 | 46.089 | 15.154 | 16.155 | 1.00 | 35.44 |
| ATOM | 5127 | C | VAL | 664 | 47.072 | 12.896 | 18.150 | 1.00 | 31.08 |
| ATOM | 5128 | O | VAL | 664 | 46.866 | 12.760 | 19.360 | 1.00 | 31.49 |
| ATOM | 5129 | N | LYS | 665 | 46.710 | 11.978 | 17.255 | 1.00 | 29.75 |
| ATOM | 5131 | CA | LYS | 665 | 45.956 | 10.788 | 17.638 | 1.00 | 28.83 |
| ATOM | 5132 | CB | LYS | 665 | 45.411 | 10.083 | 16.397 | 1.00 | 29.52 |
| ATOM | 5133 | CG | LYS | 665 | 44.242 | 10.835 | 15.797 | 1.00 | 27.21 |
| ATOM | 5134 | CD | LYS | 665 | 43.905 | 10.431 | 14.397 | 1.00 | 27.25 |
| ATOM | 5135 | CE | LYS | 665 | 42.684 | 11.228 | 13.931 | 1.00 | 28.63 |
| ATOM | 5136 | NZ | LYS | 665 | 42.266 | 10.902 | 12.545 | 1.00 | 25.33 |
| ATOM | 5140 | C | LYS | 665 | 46.718 | 9.830 | 18.537 | 1.00 | 29.03 |
| ATOM | 5141 | O | LYS | 665 | 46.152 | 8.869 | 19.046 | 1.00 | 28.37 |
| ATOM | 5142 | N | TRP | 666 | 47.994 | 10.123 | 18.765 | 1.00 | 30.40 |
| ATOM | 5144 | CA | TRP | 666 | 48.825 | 9.296 | 19.628 | 1.00 | 31.10 |
| ATOM | 5145 | CB | TRP | 666 | 50.123 | 8.906 | 18.917 | 1.00 | 29.53 |
| ATOM | 5146 | CG | TRP | 666 | 49.946 | 7.781 | 17.966 | 1.00 | 27.03 |
| ATOM | 5147 | CD2 | TRP | 666 | 49.407 | 7.853 | 16.638 | 1.00 | 25.06 |
| ATOM | 5148 | CE2 | TRP | 666 | 49.418 | 6.546 | 16.116 | 1.00 | 23.83 |
| ATOM | 5149 | CE3 | TRP | 666 | 48.924 | 8.899 | 15.835 | 1.00 | 26.08 |
| ATOM | 5150 | CD1 | TRP | 666 | 50.257 | 6.475 | 18.186 | 1.00 | 20.75 |
| ATOM | 5151 | NE1 | TRP | 666 | 49.937 | 5.729 | 17.086 | 1.00 | 24.92 |
| ATOM | 5153 | CZ2 | TRP | 666 | 48.962 | 6.245 | 14.832 | 1.00 | 23.95 |
| ATOM | 5154 | CZ3 | TRP | 666 | 48.466 | 8.604 | 14.548 | 1.00 | 29.09 |
| ATOM | 5155 | CH2 | TRP | 666 | 48.491 | 7.282 | 14.060 | 1.00 | 29.22 |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5156 | C | TRP | 666 | 49.174 | 10.049 | 20.896 | 1.00 | 33.20 |
| ATOM | 5157 | O | TRP | 666 | 49.701 | 9.469 | 21.849 | 1.00 | 34.39 |
| ATOM | 5158 | N | MET | 667 | 48.862 | 11.340 | 20.910 | 1.00 | 34.82 |
| ATOM | 5160 | CA | MET | 667 | 49.169 | 12.175 | 22.056 | 1.00 | 36.31 |
| ATOM | 5161 | CB | MET | 667 | 49.205 | 13.645 | 21.651 | 1.00 | 40.08 |
| ATOM | 5162 | CG | MET | 667 | 50.475 | 14.047 | 20.931 | 1.00 | 42.41 |
| ATOM | 5163 | SD | MET | 667 | 50.555 | 15.818 | 20.713 | 1.00 | 51.31 |
| ATOM | 5164 | CE | MET | 667 | 50.957 | 15.928 | 18.949 | 1.00 | 45.44 |
| ATOM | 5165 | C | MET | 667 | 48.299 | 12.003 | 23.287 | 1.00 | 37.81 |
| ATOM | 5166 | O | MET | 667 | 47.081 | 11.871 | 23.195 | 1.00 | 38.91 |
| ATOM | 5167 | N | ALA | 668 | 48.958 | 11.964 | 24.442 | 1.00 | 36.47 |
| ATOM | 5169 | CA | ALA | 668 | 48.286 | 11.846 | 25.718 | 1.00 | 37.06 |
| ATOM | 5170 | CB | ALA | 668 | 49.308 | 11.654 | 26.835 | 1.00 | 35.76 |
| ATOM | 5171 | C | ALA | 668 | 47.548 | 13.161 | 25.893 | 1.00 | 38.76 |
| ATOM | 5172 | O | ALA | 668 | 48.000 | 14.201 | 25.414 | 1.00 | 38.04 |
| ATOM | 5173 | N | PRO | 669 | 46.416 | 13.142 | 26.608 | 1.00 | 41.60 |
| ATOM | 5174 | CD | PRO | 669 | 45.819 | 11.981 | 27.282 | 1.00 | 41.64 |
| ATOM | 5175 | CA | PRO | 669 | 45.614 | 14.347 | 26.841 | 1.00 | 43.25 |
| ATOM | 5176 | CB | PRO | 669 | 44.478 | 13.827 | 27.718 | 1.00 | 45.08 |
| ATOM | 5177 | CG | PRO | 669 | 44.383 | 12.368 | 27.325 | 1.00 | 44.04 |
| ATOM | 5178 | C | PRO | 669 | 46.390 | 15.486 | 27.526 | 1.00 | 44.68 |
| ATOM | 5179 | O | PRO | 669 | 46.304 | 16.644 | 27.111 | 1.00 | 43.79 |
| ATOM | 5180 | N | GLU | 670 | 47.135 | 15.164 | 28.580 | 1.00 | 44.29 |
| ATOM | 5182 | CA | GLU | 670 | 47.905 | 16.195 | 29.266 | 1.00 | 45.36 |
| ATOM | 5183 | CB | GLU | 670 | 48.596 | 15.637 | 30.509 | 1.00 | 46.97 |
| ATOM | 5184 | CG | GLU | 670 | 49.858 | 14.819 | 30.243 | 1.00 | 50.04 |
| ATOM | 5185 | CD | GLU | 670 | 49.588 | 13.345 | 30.070 | 1.00 | 51.35 |
| ATOM | 5186 | OE1 | GLU | 670 | 50.512 | 12.552 | 30.327 | 1.00 | 50.99 |
| ATOM | 5187 | OE2 | GLU | 670 | 48.458 | 12.975 | 29.700 | 1.00 | 52.70 |
| ATOM | 5188 | C | GLU | 670 | 48.942 | 16.802 | 28.320 | 1.00 | 45.63 |
| ATOM | 5189 | O | GLU | 670 | 49.174 | 18.006 | 28.340 | 1.00 | 44.75 |
| ATOM | 5190 | N | ALA | 671 | 49.546 | 15.962 | 27.482 | 1.00 | 46.18 |
| ATOM | 5192 | CA | ALA | 671 | 50.555 | 16.406 | 26.531 | 1.00 | 46.44 |
| ATOM | 5193 | CB | ALA | 671 | 51.218 | 15.203 | 25.860 | 1.00 | 43.27 |
| ATOM | 5194 | C | ALA | 671 | 49.931 | 17.313 | 25.483 | 1.00 | 47.85 |
| ATOM | 5195 | O | ALA | 671 | 50.485 | 18.355 | 25.150 | 1.00 | 47.61 |
| ATOM | 5196 | N | LEU | 672 | 48.748 | 16.928 | 25.018 | 1.00 | 51.40 |
| ATOM | 5198 | CA | LEU | 672 | 48.010 | 17.657 | 23.990 | 1.00 | 54.25 |
| ATOM | 5199 | CB | LEU | 672 | 46.996 | 16.705 | 23.346 | 1.00 | 55.60 |
| ATOM | 5200 | CG | LEU | 672 | 46.202 | 17.113 | 22.105 | 1.00 | 58.92 |
| ATOM | 5201 | CD1 | LEU | 672 | 47.114 | 17.425 | 20.932 | 1.00 | 58.60 |
| ATOM | 5202 | CD2 | LEU | 672 | 45.269 | 15.977 | 21.753 | 1.00 | 60.32 |
| ATOM | 5203 | C | LEU | 672 | 47.315 | 18.925 | 24.514 | 1.00 | 55.91 |
| ATOM | 5204 | O | LEU | 672 | 47.289 | 19.958 | 23.837 | 1.00 | 55.72 |
| ATOM | 5205 | N | PHE | 673 | 46.782 | 18.846 | 25.730 | 1.00 | 57.88 |
| ATOM | 5207 | CA | PHE | 673 | 46.089 | 19.977 | 26.342 | 1.00 | 60.07 |
| ATOM | 5208 | CB | PHE | 673 | 44.873 | 19.484 | 27.127 | 1.00 | 57.08 |
| ATOM | 5209 | CG | PHE | 673 | 43.876 | 18.742 | 26.290 | 1.00 | 56.39 |
| ATOM | 5210 | CD1 | PHE | 673 | 43.191 | 17.653 | 26.813 | 1.00 | 57.67 |
| ATOM | 5211 | CD2 | PHE | 673 | 43.633 | 19.116 | 24.970 | 1.00 | 55.36 |
| ATOM | 5212 | CE1 | PHE | 673 | 42.281 | 16.939 | 26.036 | 1.00 | 57.42 |
| ATOM | 5213 | CE2 | PHE | 673 | 42.724 | 18.410 | 24.183 | 1.00 | 55.91 |
| ATOM | 5214 | CZ | PHE | 673 | 42.049 | 17.317 | 24.720 | 1.00 | 56.42 |
| ATOM | 5215 | C | PHE | 673 | 46.974 | 20.854 | 27.238 | 1.00 | 63.00 |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5216 | O | PHE | 673 | 46.926 | 22.085 | 27.155 | 1.00 | 65.31 |
| ATOM | 5217 | N | ASP | 674 | 47.786 | 20.223 | 28.081 | 1.00 | 64.08 |
| ATOM | 5219 | CA | ASP | 674 | 48.656 | 20.954 | 28.999 | 1.00 | 64.97 |
| ATOM | 5220 | CB | ASP | 674 | 48.545 | 20.375 | 30.409 | 1.00 | 65.13 |
| ATOM | 5221 | CG | ASP | 674 | 47.128 | 20.358 | 30.923 | 1.00 | 67.33 |
| ATOM | 5222 | OD1 | ASP | 674 | 46.684 | 19.283 | 31.372 | 1.00 | 66.68 |
| ATOM | 5223 | OD2 | ASP | 674 | 46.462 | 21.416 | 30.869 | 1.00 | 69.20 |
| ATOM | 5224 | C | ASP | 674 | 50.132 | 20.971 | 28.603 | 1.00 | 66.38 |
| ATOM | 5225 | O | ASP | 674 | 50.984 | 21.304 | 29.434 | 1.00 | 68.44 |
| ATOM | 5226 | N | ARG | 675 | 50.441 | 20.585 | 27.365 | 1.00 | 65.68 |
| ATOM | 5228 | CA | ARG | 675 | 51.829 | 20.550 | 26.883 | 1.00 | 63.71 |
| ATOM | 5229 | CB | ARG | 675 | 52.321 | 21.970 | 26.576 | 1.00 | 63.67 |
| ATOM | 5230 | CG | ARG | 675 | 51.491 | 22.685 | 25.531 | 1.00 | 67.65 |
| ATOM | 5231 | CD | ARG | 675 | 52.094 | 24.034 | 25.146 | 1.00 | 73.20 |
| ATOM | 5232 | NE | ARG | 675 | 53.382 | 23.911 | 24.457 | 1.00 | 74.09 |
| ATOM | 5234 | CZ | ARG | 675 | 54.159 | 24.939 | 24.122 | 1.00 | 73.41 |
| ATOM | 5235 | NH1 | ARG | 675 | 53.788 | 26.182 | 24.408 | 1.00 | 72.90 |
| ATOM | 5238 | NH2 | ARG | 675 | 55.324 | 24.720 | 23.524 | 1.00 | 71.96 |
| ATOM | 5241 | C | ARG | 675 | 52.780 | 19.864 | 27.876 | 1.00 | 61.41 |
| ATOM | 5242 | O | ARG | 675 | 53.960 | 20.208 | 27.966 | 1.00 | 62.62 |
| ATOM | 5243 | N | ILE | 676 | 52.248 | 18.903 | 28.627 | 1.00 | 59.15 |
| ATOM | 5245 | CA | ILE | 676 | 53.016 | 18.162 | 29.623 | 1.00 | 56.88 |
| ATOM | 5246 | CB | ILE | 676 | 52.175 | 17.904 | 30.891 | 1.00 | 56.26 |
| ATOM | 5247 | CG2 | ILE | 676 | 52.871 | 16.904 | 31.807 | 1.00 | 53.11 |
| ATOM | 5248 | CG1 | ILE | 676 | 51.920 | 19.224 | 31.614 | 1.00 | 57.86 |
| ATOM | 5249 | CD1 | ILE | 676 | 51.038 | 19.096 | 32.835 | 1.00 | 61.05 |
| ATOM | 5250 | C | ILE | 676 | 53.494 | 16.828 | 29.070 | 1.00 | 56.58 |
| ATOM | 5251 | O | ILE | 676 | 52.727 | 15.869 | 28.985 | 1.00 | 58.12 |
| ATOM | 5252 | N | TYR | 677 | 54.760 | 16.773 | 28.680 | 1.00 | 54.34 |
| ATOM | 5254 | CA | TYR | 677 | 55.340 | 15.556 | 28.143 | 1.00 | 51.14 |
| ATOM | 5255 | CB | TYR | 677 | 56.240 | 15.868 | 26.954 | 1.00 | 52.37 |
| ATOM | 5256 | CG | TYR | 677 | 55.488 | 16.315 | 25.719 | 1.00 | 56.21 |
| ATOM | 5257 | CD1 | TYR | 677 | 55.187 | 17.660 | 25.512 | 1.00 | 56.78 |
| ATOM | 5258 | CE1 | TYR | 677 | 54.534 | 18.086 | 24.353 | 1.00 | 57.54 |
| ATOM | 5259 | CD2 | TYR | 677 | 55.113 | 15.395 | 24.738 | 1.00 | 57.82 |
| ATOM | 5260 | CE2 | TYR | 677 | 54.458 | 15.809 | 23.571 | 1.00 | 59.32 |
| ATOM | 5261 | CZ | TYR | 677 | 54.177 | 17.159 | 23.385 | 1.00 | 59.59 |
| ATOM | 5262 | OH | TYR | 677 | 53.557 | 17.589 | 22.230 | 1.00 | 60.15 |
| ATOM | 5264 | C | TYR | 677 | 56.124 | 14.854 | 29.224 | 1.00 | 48.64 |
| ATOM | 5265 | O | TYR | 677 | 57.040 | 15.430 | 29.812 | 1.00 | 50.45 |
| ATOM | 5266 | N | THR | 678 | 55.733 | 13.621 | 29.510 | 1.00 | 44.59 |
| ATOM | 5268 | CA | THR | 678 | 56.397 | 12.834 | 30.524 | 1.00 | 42.21 |
| ATOM | 5269 | CB | THR | 678 | 55.524 | 12.726 | 31.791 | 1.00 | 43.55 |
| ATOM | 5270 | OG1 | THR | 678 | 54.302 | 12.045 | 31.475 | 1.00 | 47.42 |
| ATOM | 5272 | CG2 | THR | 678 | 55.190 | 14.105 | 32.327 | 1.00 | 48.74 |
| ATOM | 5273 | C | THR | 678 | 56.634 | 11.432 | 29.992 | 1.00 | 39.94 |
| ATOM | 5274 | O | THR | 678 | 56.207 | 11.085 | 28.892 | 1.00 | 39.34 |
| ATOM | 5275 | N | HIS | 679 | 57.312 | 10.616 | 30.784 | 1.00 | 38.54 |
| ATOM | 5277 | CA | HIS | 679 | 57.532 | 9.248 | 30.390 | 1.00 | 38.29 |
| ATOM | 5278 | CB | HIS | 679 | 58.441 | 8.546 | 31.391 | 1.00 | 39.51 |
| ATOM | 5279 | CG | HIS | 679 | 59.869 | 8.997 | 31.331 | 1.00 | 43.13 |
| ATOM | 5280 | CD2 | HIS | 679 | 60.630 | 9.668 | 32.233 | 1.00 | 43.49 |
| ATOM | 5281 | ND1 | HIS | 679 | 60.694 | 8.726 | 30.263 | 1.00 | 43.00 |
| ATOM | 5283 | CE1 | HIS | 679 | 61.903 | 9.201 | 30.510 | 1.00 | 43.62 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5284 | NE2 | HIS | 679 | 61.889 | 9.778 | 31.695 | 1.00 | 44.68 |
| ATOM | 5286 | C | HIS | 679 | 56.147 | 8.599 | 30.359 | 1.00 | 39.42 |
| ATOM | 5287 | O | HIS | 679 | 55.898 | 7.667 | 29.593 | 1.00 | 40.00 |
| ATOM | 5288 | N | GLN | 680 | 55.228 | 9.156 | 31.142 | 1.00 | 38.96 |
| ATOM | 5290 | CA | GLN | 680 | 53.867 | 8.649 | 31.209 | 1.00 | 38.84 |
| ATOM | 5291 | CB | GLN | 680 | 53.214 | 9.010 | 32.543 | 1.00 | 40.90 |
| ATOM | 5292 | CG | GLN | 680 | 53.835 | 8.278 | 33.732 | 1.00 | 44.42 |
| ATOM | 5293 | CD | GLN | 680 | 53.677 | 6.756 | 33.660 | 1.00 | 44.47 |
| ATOM | 5294 | OE1 | GLN | 680 | 52.595 | 6.225 | 33.908 | 1.00 | 45.52 |
| ATOM | 5295 | NE2 | GLN | 680 | 54.767 | 6.050 | 33.348 | 1.00 | 42.06 |
| ATOM | 5298 | C | GLN | 680 | 53.013 | 9.099 | 30.036 | 1.00 | 38.25 |
| ATOM | 5299 | O | GLN | 680 | 51.968 | 8.505 | 29.758 | 1.00 | 39.27 |
| ATOM | 5300 | N | SER | 681 | 53.427 | 10.155 | 29.349 | 1.00 | 37.00 |
| ATOM | 5302 | CA | SER | 681 | 52.665 | 10.571 | 28.182 | 1.00 | 38.02 |
| ATOM | 5303 | CB | SER | 681 | 52.929 | 12.034 | 27.813 | 1.00 | 40.29 |
| ATOM | 5304 | OG | SER | 681 | 54.307 | 12.286 | 27.620 | 1.00 | 47.29 |
| ATOM | 5306 | C | SER | 681 | 53.066 | 9.620 | 27.051 | 1.00 | 37.43 |
| ATOM | 5307 | O | SER | 681 | 52.289 | 9.366 | 26.136 | 1.00 | 37.86 |
| ATOM | 5308 | N | ASP | 682 | 54.281 | 9.077 | 27.162 | 1.00 | 35.23 |
| ATOM | 5310 | CA | ASP | 682 | 54.800 | 8.106 | 26.205 | 1.00 | 33.24 |
| ATOM | 5311 | CB | ASP | 682 | 56.284 | 7.820 | 26.464 | 1.00 | 31.85 |
| ATOM | 5312 | CG | ASP | 682 | 57.224 | 8.732 | 25.677 | 1.00 | 34.18 |
| ATOM | 5313 | OD1 | ASP | 682 | 58.445 | 8.537 | 25.826 | 1.00 | 31.79 |
| ATOM | 5314 | OD2 | ASP | 682 | 56.763 | 9.620 | 24.908 | 1.00 | 29.15 |
| ATOM | 5315 | C | ASP | 682 | 54.015 | 6.810 | 26.374 | 1.00 | 31.52 |
| ATOM | 5316 | O | ASP | 682 | 53.788 | 6.087 | 25.411 | 1.00 | 31.93 |
| ATOM | 5317 | N | VAL | 683 | 53.653 | 6.499 | 27.617 | 1.00 | 33.14 |
| ATOM | 5319 | CA | VAL | 683 | 52.879 | 5.293 | 27.935 | 1.00 | 32.79 |
| ATOM | 5320 | CB | VAL | 683 | 52.725 | 5.095 | 29.478 | 1.00 | 34.56 |
| ATOM | 5321 | CG1 | VAL | 683 | 51.653 | 4.059 | 29.790 | 1.00 | 32.39 |
| ATOM | 5322 | CG2 | VAL | 683 | 54.050 | 4.649 | 30.088 | 1.00 | 28.08 |
| ATOM | 5323 | C | VAL | 683 | 51.506 | 5.338 | 27.245 | 1.00 | 31.45 |
| ATOM | 5324 | O | VAL | 683 | 51.008 | 4.311 | 26.779 | 1.00 | 30.37 |
| ATOM | 5325 | N | TRP | 684 | 50.919 | 6.531 | 27.147 | 1.00 | 31.04 |
| ATOM | 5327 | CA | TRP | 684 | 49.638 | 6.686 | 26.464 | 1.00 | 31.23 |
| ATOM | 5328 | CB | TRP | 684 | 49.158 | 8.137 | 26.525 | 1.00 | 34.14 |
| ATOM | 5329 | CG | TRP | 684 | 47.913 | 8.423 | 25.694 | 1.00 | 37.17 |
| ATOM | 5330 | CD2 | TRP | 684 | 46.573 | 8.593 | 26.187 | 1.00 | 38.61 |
| ATOM | 5331 | CE2 | TRP | 684 | 45.755 | 8.888 | 25.064 | 1.00 | 37.91 |
| ATOM | 5332 | CE3 | TRP | 684 | 45.978 | 8.528 | 27.452 | 1.00 | 37.63 |
| ATOM | 5333 | CD1 | TRP | 684 | 47.850 | 8.612 | 24.337 | 1.00 | 37.39 |
| ATOM | 5334 | NE1 | TRP | 684 | 46.560 | 8.894 | 23.956 | 1.00 | 34.76 |
| ATOM | 5336 | CZ2 | TRP | 684 | 44.380 | 9.118 | 25.181 | 1.00 | 34.79 |
| ATOM | 5337 | CZ3 | TRP | 684 | 44.611 | 8.759 | 27.563 | 1.00 | 38.53 |
| ATOM | 5338 | CH2 | TRP | 684 | 43.830 | 9.048 | 26.428 | 1.00 | 37.59 |
| ATOM | 5339 | C | TRP | 684 | 49.876 | 6.294 | 25.013 | 1.00 | 29.99 |
| ATOM | 5340 | O | TRP | 684 | 49.254 | 5.356 | 24.503 | 1.00 | 30.82 |
| ATOM | 5341 | N | SER | 685 | 50.815 | 6.992 | 24.380 | 1.00 | 28.28 |
| ATOM | 5343 | CA | SER | 685 | 51.174 | 6.738 | 22.986 | 1.00 | 27.54 |
| ATOM | 5344 | CB | SER | 685 | 52.444 | 7.504 | 22.631 | 1.00 | 26.69 |
| ATOM | 5345 | OG | SER | 685 | 52.355 | 8.874 | 22.986 | 1.00 | 32.15 |
| ATOM | 5347 | C | SER | 685 | 51.399 | 5.249 | 22.737 | 1.00 | 26.41 |
| ATOM | 5348 | O | SER | 685 | 50.968 | 4.709 | 21.713 | 1.00 | 29.52 |
| ATOM | 5349 | N | PHE | 686 | 52.065 | 4.582 | 23.676 | 1.00 | 26.47 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5351 | CA | PHE | 686 | 52.325 | 3.151 | 23.563 | 1.00 | 26.35 |
| ATOM | 5352 | CB | PHE | 686 | 53.167 | 2.668 | 24.754 | 1.00 | 25.01 |
| ATOM | 5353 | CG | PHE | 686 | 53.447 | 1.182 | 24.742 | 1.00 | 27.24 |
| ATOM | 5354 | CD1 | PHE | 686 | 54.187 | 0.600 | 23.712 | 1.00 | 24.88 |
| ATOM | 5355 | CD2 | PHE | 686 | 52.915 | 0.351 | 25.729 | 1.00 | 24.99 |
| ATOM | 5356 | CE1 | PHE | 686 | 54.389 | -0.783 | 23.655 | 1.00 | 22.77 |
| ATOM | 5357 | CE2 | PHE | 686 | 53.113 | -1.036 | 25.679 | 1.00 | 28.39 |
| ATOM | 5358 | CZ | PHE | 686 | 53.853 | -1.601 | 24.631 | 1.00 | 22.71 |
| ATOM | 5359 | C | PHE | 686 | 50.997 | 2.366 | 23.466 | 1.00 | 28.82 |
| ATOM | 5360 | O | PHE | 686 | 50.892 | 1.398 | 22.696 | 1.00 | 26.41 |
| ATOM | 5361 | N | GLY | 687 | 49.988 | 2.797 | 24.229 | 1.00 | 29.65 |
| ATOM | 5363 | CA | GLY | 687 | 48.692 | 2.134 | 24.194 | 1.00 | 29.88 |
| ATOM | 5364 | C | GLY | 687 | 48.099 | 2.158 | 22.794 | 1.00 | 29.57 |
| ATOM | 5365 | O | GLY | 687 | 47.560 | 1.165 | 22.300 | 1.00 | 30.38 |
| ATOM | 5366 | N | VAL | 688 | 48.222 | 3.310 | 22.147 | 1.00 | 29.19 |
| ATOM | 5368 | CA | VAL | 688 | 47.718 | 3.478 | 20.795 | 1.00 | 25.09 |
| ATOM | 5369 | CB | VAL | 688 | 47.747 | 4.956 | 20.359 | 1.00 | 22.52 |
| ATOM | 5370 | CG1 | VAL | 688 | 47.106 | 5.115 | 18.985 | 1.00 | 21.13 |
| ATOM | 5371 | CG2 | VAL | 688 | 47.001 | 5.810 | 21.366 | 1.00 | 22.50 |
| ATOM | 5372 | C | VAL | 688 | 48.574 | 2.636 | 19.865 | 1.00 | 23.82 |
| ATOM | 5373 | O | VAL | 688 | 48.080 | 2.132 | 18.871 | 1.00 | 25.39 |
| ATOM | 5374 | N | LEU | 689 | 49.849 | 2.463 | 20.208 | 1.00 | 24.46 |
| ATOM | 5376 | CA | LEU | 689 | 50.764 | 1.655 | 19.401 | 1.00 | 25.68 |
| ATOM | 5377 | CB | LEU | 689 | 52.222 | 1.893 | 19.834 | 1.00 | 25.93 |
| ATOM | 5378 | CG | LEU | 689 | 53.374 | 1.307 | 19.004 | 1.00 | 25.01 |
| ATOM | 5379 | CD1 | LEU | 689 | 54.655 | 2.080 | 19.257 | 1.00 | 25.86 |
| ATOM | 5380 | CD2 | LEU | 689 | 53.593 | -0.145 | 19.318 | 1.00 | 24.90 |
| ATOM | 5381 | C | LEU | 689 | 50.374 | 0.171 | 19.531 | 1.00 | 26.50 |
| ATOM | 5382 | O | LEU | 689 | 50.464 | -0.578 | 18.558 | 1.00 | 27.13 |
| ATOM | 5383 | N | LEU | 690 | 49.927 | -0.234 | 20.724 | 1.00 | 27.76 |
| ATOM | 5385 | CA | LEU | 690 | 49.481 | -1.610 | 20.980 | 1.00 | 28.59 |
| ATOM | 5386 | CB | LEU | 690 | 49.087 | -1.800 | 22.447 | 1.00 | 30.38 |
| ATOM | 5387 | CG | LEU | 690 | 50.121 | -2.065 | 23.545 | 1.00 | 29.57 |
| ATOM | 5388 | CD1 | LEU | 690 | 49.435 | -1.966 | 24.907 | 1.00 | 27.40 |
| ATOM | 5389 | CD2 | LEU | 690 | 50.744 | -3.431 | 23.360 | 1.00 | 28.79 |
| ATOM | 5390 | C | LEU | 690 | 48.242 | -1.849 | 20.134 | 1.00 | 28.77 |
| ATOM | 5391 | O | LEU | 690 | 48.055 | -2.922 | 19.573 | 1.00 | 28.07 |
| ATOM | 5392 | N | TRP | 691 | 47.383 | -0.838 | 20.075 | 1.00 | 29.58 |
| ATOM | 5394 | CA | TRP | 691 | 46.166 | -0.921 | 19.275 | 1.00 | 30.53 |
| ATOM | 5395 | CB | TRP | 691 | 45.327 | 0.349 | 19.451 | 1.00 | 28.28 |
| ATOM | 5396 | CG | TRP | 691 | 43.985 | 0.300 | 18.769 | 1.00 | 25.86 |
| ATOM | 5397 | CD2 | TRP | 691 | 43.702 | 0.689 | 17.421 | 1.00 | 23.99 |
| ATOM | 5398 | CE2 | TRP | 691 | 42.321 | 0.498 | 17.215 | 1.00 | 25.08 |
| ATOM | 5399 | CE3 | TRP | 691 | 44.487 | 1.165 | 16.367 | 1.00 | 20.88 |
| ATOM | 5400 | CD1 | TRP | 691 | 42.791 | -0.090 | 19.314 | 1.00 | 23.72 |
| ATOM | 5401 | NE1 | TRP | 691 | 41.786 | 0.031 | 18.389 | 1.00 | 26.15 |
| ATOM | 5403 | CZ2 | TRP | 691 | 41.704 | 0.788 | 15.997 | 1.00 | 25.07 |
| ATOM | 5404 | CZ3 | TRP | 691 | 43.883 | 1.448 | 15.163 | 1.00 | 22.80 |
| ATOM | 5405 | CH2 | TRP | 691 | 42.501 | 1.251 | 14.982 | 1.00 | 24.95 |
| ATOM | 5406 | C | TRP | 691 | 46.566 | -1.116 | 17.811 | 1.00 | 30.63 |
| ATOM | 5407 | O | TRP | 691 | 45.943 | -1.892 | 17.093 | 1.00 | 33.02 |
| ATOM | 5408 | N | GLU | 692 | 47.625 | -0.431 | 17.386 | 1.00 | 31.00 |
| ATOM | 5410 | CA | GLU | 692 | 48.130 | -0.545 | 16.018 | 1.00 | 29.00 |
| ATOM | 5411 | CB | GLU | 692 | 49.285 | 0.426 | 15.778 | 1.00 | 26.55 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5412 | CG | GLU | 692 | 48.873 | 1.876 | 15.651 | 1.00 | 29.90 |
| ATOM | 5413 | CD | GLU | 692 | 50.040 | 2.781 | 15.316 | 1.00 | 29.83 |
| ATOM | 5414 | OE1 | GLU | 692 | 50.770 | 3.174 | 16.247 | 1.00 | 32.18 |
| ATOM | 5415 | OE2 | GLU | 692 | 50.227 | 3.110 | 14.124 | 1.00 | 31.57 |
| ATOM | 5416 | C | GLU | 692 | 48.622 | -1.959 | 15.735 | 1.00 | 29.02 |
| ATOM | 5417 | O | GLU | 692 | 48.474 | -2.467 | 14.627 | 1.00 | 29.22 |
| ATOM | 5418 | N | ILE | 693 | 49.258 | -2.573 | 16.724 | 1.00 | 29.54 |
| ATOM | 5420 | CA | ILE | 693 | 49.766 | -3.933 | 16.555 | 1.00 | 31.01 |
| ATOM | 5421 | CB | ILE | 693 | 50.634 | -4.360 | 17.757 | 1.00 | 32.36 |
| ATOM | 5422 | CG2 | ILE | 693 | 51.006 | -5.845 | 17.641 | 1.00 | 34.39 |
| ATOM | 5423 | CG1 | ILE | 693 | 51.909 | -3.506 | 17.815 | 1.00 | 30.30 |
| ATOM | 5424 | CD1 | ILE | 693 | 52.696 | -3.693 | 19.082 | 1.00 | 25.66 |
| ATOM | 5425 | C | ILE | 693 | 48.638 | -4.939 | 16.381 | 1.00 | 30.63 |
| ATOM | 5426 | O | ILE | 693 | 48.633 | -5.738 | 15.451 | 1.00 | 31.10 |
| ATOM | 5427 | N | PHE | 694 | 47.644 | -4.858 | 17.248 | 1.00 | 32.60 |
| ATOM | 5429 | CA | PHE | 694 | 46.543 | -5.793 | 17.172 | 1.00 | 33.86 |
| ATOM | 5430 | CB | PHE | 694 | 45.938 | -5.970 | 18.563 | 1.00 | 35.66 |
| ATOM | 5431 | CG | PHE | 694 | 46.941 | -6.499 | 19.559 | 1.00 | 35.70 |
| ATOM | 5432 | CD1 | PHE | 694 | 47.460 | -5.684 | 20.556 | 1.00 | 37.18 |
| ATOM | 5433 | CD2 | PHE | 694 | 47.449 | -7.794 | 19.426 | 1.00 | 34.37 |
| ATOM | 5434 | CE1 | PHE | 694 | 48.473 | -6.150 | 21.392 | 1.00 | 36.90 |
| ATOM | 5435 | CE2 | PHE | 694 | 48.456 | -8.265 | 20.255 | 1.00 | 31.89 |
| ATOM | 5436 | CZ | PHE | 694 | 48.970 | -7.446 | 21.234 | 1.00 | 34.95 |
| ATOM | 5437 | C | PHE | 694 | 45.532 | -5.576 | 16.049 | 1.00 | 34.26 |
| ATOM | 5438 | O | PHE | 694 | 44.702 | -6.442 | 15.787 | 1.00 | 37.52 |
| ATOM | 5439 | N | THR | 695 | 45.636 | -4.441 | 15.359 | 1.00 | 32.23 |
| ATOM | 5441 | CA | THR | 695 | 44.775 | -4.160 | 14.215 | 1.00 | 28.08 |
| ATOM | 5442 | CB | THR | 695 | 44.186 | -2.728 | 14.241 | 1.00 | 25.71 |
| ATOM | 5443 | OG1 | THR | 695 | 45.237 | -1.762 | 14.228 | 1.00 | 24.94 |
| ATOM | 5445 | CG2 | THR | 695 | 43.353 | -2.528 | 15.468 | 1.00 | 23.07 |
| ATOM | 5446 | C | THR | 695 | 45.615 | -4.348 | 12.955 | 1.00 | 27.53 |
| ATOM | 5447 | O | THR | 695 | 45.166 | -4.066 | 11.845 | 1.00 | 30.89 |
| ATOM | 5448 | N | LEU | 696 | 46.833 | -4.848 | 13.145 | 1.00 | 27.73 |
| ATOM | 5450 | CA | LEU | 696 | 47.781 | -5.081 | 12.061 | 1.00 | 28.99 |
| ATOM | 5451 | CB | LEU | 696 | 47.370 | -6.297 | 11.226 | 1.00 | 27.78 |
| ATOM | 5452 | CG | LEU | 696 | 47.379 | -7.591 | 12.047 | 1.00 | 29.89 |
| ATOM | 5453 | CD1 | LEU | 696 | 47.251 | -8.823 | 11.164 | 1.00 | 29.96 |
| ATOM | 5454 | CD2 | LEU | 696 | 48.668 | -7.656 | 12.803 | 1.00 | 30.20 |
| ATOM | 5455 | C | LEU | 696 | 48.044 | -3.853 | 11.179 | 1.00 | 30.33 |
| ATOM | 5456 | O | LEU | 696 | 48.006 | -3.926 | 9.948 | 1.00 | 29.41 |
| ATOM | 5457 | N | GLY | 697 | 48.374 | -2.738 | 11.831 | 1.00 | 30.92 |
| ATOM | 5459 | CA | GLY | 697 | 48.655 | -1.503 | 11.113 | 1.00 | 30.35 |
| ATOM | 5460 | C | GLY | 697 | 47.420 | -0.650 | 10.912 | 1.00 | 30.65 |
| ATOM | 5461 | O | GLY | 697 | 47.359 | 0.178 | 10.000 | 1.00 | 30.01 |
| ATOM | 5462 | N | GLY | 698 | 46.428 | -0.836 | 11.772 | 1.00 | 30.50 |
| ATOM | 5464 | CA | GLY | 698 | 45.209 | -0.063 | 11.656 | 1.00 | 30.36 |
| ATOM | 5465 | C | GLY | 698 | 45.416 | 1.415 | 11.930 | 1.00 | 30.07 |
| ATOM | 5466 | O | GLY | 698 | 46.320 | 1.809 | 12.666 | 1.00 | 30.56 |
| ATOM | 5467 | N | SER | 699 | 44.554 | 2.228 | 11.338 | 1.00 | 29.65 |
| ATOM | 5469 | CA | SER | 699 | 44.597 | 3.674 | 11.485 | 1.00 | 28.42 |
| ATOM | 5470 | CB | SER | 699 | 44.263 | 4.324 | 10.145 | 1.00 | 24.61 |
| ATOM | 5471 | OG | SER | 699 | 43.960 | 5.693 | 10.280 | 1.00 | 31.25 |
| ATOM | 5473 | C | SER | 699 | 43.621 | 4.137 | 12.574 | 1.00 | 28.27 |
| ATOM | 5474 | O | SER | 699 | 42.406 | 3.930 | 12.474 | 1.00 | 27.14 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5475 | N | PRO | 700 | 44.160 | 4.682 | 13.675 | 1.00 | 29.29 |
| ATOM | 5476 | CD | PRO | 700 | 45.587 | 4.867 | 13.999 | 1.00 | 26.09 |
| ATOM | 5477 | CA | PRO | 700 | 43.303 | 5.155 | 14.764 | 1.00 | 29.30 |
| ATOM | 5478 | CB | PRO | 700 | 44.319 | 5.624 | 15.812 | 1.00 | 27.68 |
| ATOM | 5479 | CG | PRO | 700 | 45.531 | 5.982 | 14.985 | 1.00 | 27.85 |
| ATOM | 5480 | C | PRO | 700 | 42.413 | 6.305 | 14.306 | 1.00 | 29.71 |
| ATOM | 5481 | O | PRO | 700 | 42.800 | 7.096 | 13.446 | 1.00 | 31.38 |
| ATOM | 5482 | N | TYR | 701 | 41.204 | 6.357 | 14.854 | 1.00 | 29.51 |
| ATOM | 5484 | CA | TYR | 701 | 40.246 | 7.419 | 14.548 | 1.00 | 30.25 |
| ATOM | 5485 | CB | TYR | 701 | 40.559 | 8.647 | 15.405 | 1.00 | 33.50 |
| ATOM | 5486 | CG | TYR | 701 | 40.321 | 8.413 | 16.866 | 1.00 | 37.84 |
| ATOM | 5487 | CD1 | TYR | 701 | 41.323 | 8.638 | 17.803 | 1.00 | 40.05 |
| ATOM | 5488 | CE1 | TYR | 701 | 41.092 | 8.412 | 19.158 | 1.00 | 42.28 |
| ATOM | 5489 | CD2 | TYR | 701 | 39.084 | 7.965 | 17.310 | 1.00 | 41.54 |
| ATOM | 5490 | CE2 | TYR | 701 | 38.845 | 7.738 | 18.653 | 1.00 | 43.70 |
| ATOM | 5491 | CZ | TYR | 701 | 39.845 | 7.963 | 19.574 | 1.00 | 42.63 |
| ATOM | 5492 | OH | TYR | 701 | 39.584 | 7.716 | 20.907 | 1.00 | 45.31 |
| ATOM | 5494 | C | TYR | 701 | 40.173 | 7.829 | 13.088 | 1.00 | 28.45 |
| ATOM | 5495 | O | TYR | 701 | 40.356 | 9.001 | 12.760 | 1.00 | 29.03 |
| ATOM | 5496 | N | PRO | 702 | 39.901 | 6.867 | 12.191 | 1.00 | 28.05 |
| ATOM | 5497 | CD | PRO | 702 | 39.671 | 5.430 | 12.417 | 1.00 | 26.90 |
| ATOM | 5498 | CA | PRO | 702 | 39.815 | 7.181 | 10.764 | 1.00 | 27.48 |
| ATOM | 5499 | CB | PRO | 702 | 39.610 | 5.807 | 10.119 | 1.00 | 27.06 |
| ATOM | 5500 | CG | PRO | 702 | 38.923 | 5.036 | 11.169 | 1.00 | 28.28 |
| ATOM | 5501 | C | PRO | 702 | 38.689 | 8.145 | 10.440 | 1.00 | 26.81 |
| ATOM | 5502 | O | PRO | 702 | 37.554 | 7.953 | 10.865 | 1.00 | 26.26 |
| ATOM | 5503 | N | GLY | 703 | 39.035 | 9.192 | 9.693 | 1.00 | 28.48 |
| ATOM | 5505 | CA | GLY | 703 | 38.085 | 10.217 | 9.295 | 1.00 | 26.54 |
| ATOM | 5506 | C | GLY | 703 | 37.862 | 11.285 | 10.351 | 1.00 | 28.03 |
| ATOM | 5507 | O | GLY | 703 | 37.110 | 12.231 | 10.108 | 1.00 | 28.93 |
| ATOM | 5508 | N | VAL | 704 | 38.518 | 11.149 | 11.505 | 1.00 | 28.16 |
| ATOM | 5510 | CA | VAL | 704 | 38.369 | 12.081 | 12.619 | 1.00 | 29.55 |
| ATOM | 5511 | CB | VAL | 704 | 38.473 | 11.360 | 13.984 | 1.00 | 28.50 |
| ATOM | 5512 | CG1 | VAL | 704 | 38.330 | 12.350 | 15.135 | 1.00 | 28.07 |
| ATOM | 5513 | CG2 | VAL | 704 | 37.403 | 10.295 | 14.091 | 1.00 | 29.78 |
| ATOM | 5514 | C | VAL | 704 | 39.375 | 13.227 | 12.588 | 1.00 | 32.00 |
| ATOM | 5515 | O | VAL | 704 | 40.578 | 13.028 | 12.758 | 1.00 | 33.85 |
| ATOM | 5516 | N | PRO | 705 | 38.888 | 14.446 | 12.336 | 1.00 | 33.56 |
| ATOM | 5517 | CD | PRO | 705 | 37.512 | 14.763 | 11.906 | 1.00 | 33.69 |
| ATOM | 5518 | CA | PRO | 705 | 39.745 | 15.628 | 12.280 | 1.00 | 32.65 |
| ATOM | 5519 | CB | PRO | 705 | 38.863 | 16.647 | 11.569 | 1.00 | 34.10 |
| ATOM | 5520 | CG | PRO | 705 | 37.478 | 16.256 | 12.021 | 1.00 | 36.38 |
| ATOM | 5521 | C | PRO | 705 | 40.164 | 16.081 | 13.668 | 1.00 | 33.22 |
| ATOM | 5522 | O | PRO | 705 | 39.549 | 15.708 | 14.668 | 1.00 | 33.26 |
| ATOM | 5523 | N | VAL | 706 | 41.198 | 16.912 | 13.710 | 1.00 | 34.61 |
| ATOM | 5525 | CA | VAL | 706 | 41.764 | 17.417 | 14.954 | 1.00 | 37.72 |
| ATOM | 5526 | CB | VAL | 706 | 42.803 | 18.527 | 14.673 | 1.00 | 39.14 |
| ATOM | 5527 | CG1 | VAL | 706 | 43.483 | 18.941 | 15.957 | 1.00 | 39.12 |
| ATOM | 5528 | CG2 | VAL | 706 | 43.836 | 18.038 | 13.670 | 1.00 | 41.07 |
| ATOM | 5529 | C | VAL | 706 | 40.740 | 17.934 | 15.969 | 1.00 | 38.70 |
| ATOM | 5530 | O | VAL | 706 | 40.761 | 17.536 | 17.136 | 1.00 | 38.42 |
| ATOM | 5531 | N | GLU | 707 | 39.834 | 18.796 | 15.517 | 1.00 | 40.43 |
| ATOM | 5533 | CA | GLU | 707 | 38.823 | 19.375 | 16.395 | 1.00 | 40.66 |
| ATOM | 5534 | CB | GLU | 707 | 37.973 | 20.379 | 15.621 | 1.00 | 43.40 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5535 | C | GLU | 707 | 37.940 | 18.316 | 17.028 | 1.00 | 41.03 |
| ATOM | 5536 | O | GLU | 707 | 37.642 | 18.370 | 18.231 | 1.00 | 41.52 |
| ATOM | 5537 | N | GLU | 708 | 37.560 | 17.327 | 16.224 | 1.00 | 41.62 |
| ATOM | 5539 | CA | GLU | 708 | 36.708 | 16.243 | 16.700 | 1.00 | 41.06 |
| ATOM | 5540 | CB | GLU | 708 | 36.179 | 15.425 | 15.523 | 1.00 | 45.19 |
| ATOM | 5541 | CG | GLU | 708 | 35.281 | 16.221 | 14.571 | 1.00 | 48.74 |
| ATOM | 5542 | CD | GLU | 708 | 34.063 | 16.825 | 15.258 | 1.00 | 57.18 |
| ATOM | 5543 | OE1 | GLU | 708 | 33.523 | 16.203 | 16.207 | 1.00 | 54.30 |
| ATOM | 5544 | OE2 | GLU | 708 | 33.646 | 17.934 | 14.837 | 1.00 | 61.76 |
| ATOM | 5545 | C | GLU | 708 | 37.443 | 15.363 | 17.694 | 1.00 | 38.39 |
| ATOM | 5546 | O | GLU | 708 | 36.867 | 14.927 | 18.696 | 1.00 | 36.76 |
| ATOM | 5547 | N | LEU | 709 | 38.725 | 15.131 | 17.434 | 1.00 | 37.78 |
| ATOM | 5549 | CA | LEU | 709 | 39.555 | 14.327 | 18.324 | 1.00 | 38.13 |
| ATOM | 5550 | CB | LEU | 709 | 41.007 | 14.255 | 17.820 | 1.00 | 35.45 |
| ATOM | 5551 | CG | LEU | 709 | 41.984 | 13.560 | 18.786 | 1.00 | 35.57 |
| ATOM | 5552 | CD1 | LEU | 709 | 41.825 | 12.049 | 18.729 | 1.00 | 32.33 |
| ATOM | 5553 | CD2 | LEU | 709 | 43.407 | 13.965 | 18.484 | 1.00 | 31.98 |
| ATOM | 5554 | C | LEU | 709 | 39.550 | 14.946 | 19.716 | 1.00 | 38.31 |
| ATOM | 5555 | O | LEU | 709 | 39.362 | 14.250 | 20.717 | 1.00 | 38.16 |
| ATOM | 5556 | N | PHE | 710 | 39.776 | 16.254 | 19.770 | 1.00 | 40.09 |
| ATOM | 5558 | CA | PHE | 710 | 39.807 | 16.973 | 21.036 | 1.00 | 43.61 |
| ATOM | 5559 | CB | PHE | 710 | 39.997 | 18.475 | 20.797 | 1.00 | 48.22 |
| ATOM | 5560 | CG | PHE | 710 | 41.328 | 18.834 | 20.192 | 1.00 | 51.77 |
| ATOM | 5561 | CD1 | PHE | 710 | 42.395 | 17.939 | 20.231 | 1.00 | 52.94 |
| ATOM | 5562 | CD2 | PHE | 710 | 41.513 | 20.072 | 19.579 | 1.00 | 53.99 |
| ATOM | 5563 | CE1 | PHE | 710 | 43.632 | 18.275 | 19.679 | 1.00 | 56.48 |
| ATOM | 5564 | CE2 | PHE | 710 | 42.746 | 20.422 | 19.021 | 1.00 | 55.72 |
| ATOM | 5565 | CZ | PHE | 710 | 43.807 | 19.517 | 19.069 | 1.00 | 57.84 |
| ATOM | 5566 | C | PHE | 710 | 38.519 | 16.726 | 21.796 | 1.00 | 43.35 |
| ATOM | 5567 | O | PHE | 710 | 38.539 | 16.424 | 22.989 | 1.00 | 43.22 |
| ATOM | 5568 | N | LYS | 711 | 37.399 | 16.804 | 21.083 | 1.00 | 44.68 |
| ATOM | 5570 | CA | LYS | 711 | 36.095 | 16.587 | 21.690 | 1.00 | 43.47 |
| ATOM | 5571 | CB | LYS | 711 | 34.977 | 16.878 | 20.687 | 1.00 | 44.33 |
| ATOM | 5572 | CG | LYS | 711 | 33.601 | 16.765 | 21.299 | 1.00 | 47.63 |
| ATOM | 5573 | CD | LYS | 711 | 32.510 | 17.206 | 20.362 | 1.00 | 49.97 |
| ATOM | 5574 | CE | LYS | 711 | 31.158 | 16.873 | 20.960 | 1.00 | 51.70 |
| ATOM | 5575 | NZ | LYS | 711 | 30.038 | 17.412 | 20.150 | 1.00 | 57.55 |
| ATOM | 5579 | C | LYS | 711 | 35.986 | 15.173 | 22.261 | 1.00 | 42.72 |
| ATOM | 5580 | O | LYS | 711 | 35.589 | 14.999 | 23.420 | 1.00 | 41.16 |
| ATOM | 5581 | N | LEU | 712 | 36.392 | 14.176 | 21.471 | 1.00 | 42.52 |
| ATOM | 5583 | CA | LEU | 712 | 36.361 | 12.770 | 21.898 | 1.00 | 42.52 |
| ATOM | 5584 | CB | LEU | 712 | 36.922 | 11.843 | 20.809 | 1.00 | 41.56 |
| ATOM | 5585 | CG | LEU | 712 | 36.090 | 11.528 | 19.560 | 1.00 | 41.87 |
| ATOM | 5586 | CD1 | LEU | 712 | 36.902 | 10.620 | 18.636 | 1.00 | 36.28 |
| ATOM | 5587 | CD2 | LEU | 712 | 34.760 | 10.868 | 19.951 | 1.00 | 37.19 |
| ATOM | 5588 | C | LEU | 712 | 37.158 | 12.564 | 23.180 | 1.00 | 42.34 |
| ATOM | 5589 | O | LEU | 712 | 36.697 | 11.886 | 24.107 | 1.00 | 40.77 |
| ATOM | 5590 | N | LEU | 713 | 38.366 | 13.121 | 23.208 | 1.00 | 42.68 |
| ATOM | 5592 | CA | LEU | 713 | 39.240 | 13.025 | 24.371 | 1.00 | 44.05 |
| ATOM | 5593 | CB | LEU | 713 | 40.581 | 13.710 | 24.100 | 1.00 | 45.45 |
| ATOM | 5594 | CG | LEU | 713 | 41.418 | 13.114 | 22.963 | 1.00 | 44.78 |
| ATOM | 5595 | CD1 | LEU | 713 | 42.676 | 13.945 | 22.750 | 1.00 | 41.89 |
| ATOM | 5596 | CD2 | LEU | 713 | 41.757 | 11.660 | 23.282 | 1.00 | 43.21 |
| ATOM | 5597 | C | LEU | 713 | 38.571 | 13.654 | 25.591 | 1.00 | 44.66 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5598 | O | LEU | 713 | 38.562 | 13.051 | 26.662 | 1.00 | 45.70 |
| ATOM | 5599 | N | LYS | 714 | 37.980 | 14.839 | 25.418 | 1.00 | 43.05 |
| ATOM | 5601 | CA | LYS | 714 | 37.300 | 15.510 | 26.524 | 1.00 | 42.19 |
| ATOM | 5602 | CB | LYS | 714 | 36.884 | 16.921 | 26.127 | 1.00 | 42.41 |
| ATOM | 5603 | CG | LYS | 714 | 38.076 | 17.828 | 25.918 | 1.00 | 46.10 |
| ATOM | 5604 | CD | LYS | 714 | 37.684 | 19.259 | 25.589 | 1.00 | 49.86 |
| ATOM | 5605 | CE | LYS | 714 | 38.939 | 20.097 | 25.292 | 1.00 | 52.55 |
| ATOM | 5606 | NZ | LYS | 714 | 39.889 | 20.148 | 26.459 | 1.00 | 50.17 |
| ATOM | 5610 | C | LYS | 714 | 36.104 | 14.728 | 27.054 | 1.00 | 42.39 |
| ATOM | 5611 | O | LYS | 714 | 35.767 | 14.824 | 28.237 | 1.00 | 43.44 |
| ATOM | 5612 | N | GLU | 715 | 35.480 | 13.934 | 26.192 | 1.00 | 40.44 |
| ATOM | 5614 | CA | GLU | 715 | 34.342 | 13.118 | 26.593 | 1.00 | 37.90 |
| ATOM | 5615 | CB | GLU | 715 | 33.408 | 12.893 | 25.411 | 1.00 | 39.54 |
| ATOM | 5616 | CG | GLU | 715 | 32.800 | 14.174 | 24.846 | 1.00 | 45.20 |
| ATOM | 5617 | CD | GLU | 715 | 32.032 | 13.936 | 23.563 | 1.00 | 47.85 |
| ATOM | 5618 | OE1 | GLU | 715 | 32.409 | 13.008 | 22.810 | 1.00 | 50.00 |
| ATOM | 5619 | OE2 | GLU | 715 | 31.061 | 14.677 | 23.304 | 1.00 | 50.41 |
| ATOM | 5620 | C | GLU | 715 | 34.793 | 11.773 | 27.157 | 1.00 | 37.31 |
| ATOM | 5621 | O | GLU | 715 | 33.970 | 10.907 | 27.450 | 1.00 | 36.79 |
| ATOM | 5622 | N | GLY | 716 | 36.102 | 11.585 | 27.286 | 1.00 | 36.60 |
| ATOM | 5624 | CA | GLY | 716 | 36.623 | 10.336 | 27.819 | 1.00 | 37.11 |
| ATOM | 5625 | C | GLY | 716 | 36.503 | 9.140 | 26.887 | 1.00 | 38.30 |
| ATOM | 5626 | O | GLY | 716 | 36.603 | 7.994 | 27.340 | 1.00 | 36.84 |
| ATOM | 5627 | N | HIS | 717 | 36.307 | 9.404 | 25.592 | 1.00 | 40.24 |
| ATOM | 5629 | CA | HIS | 717 | 36.167 | 8.353 | 24.579 | 1.00 | 42.63 |
| ATOM | 5630 | CB | HIS | 717 | 35.800 | 8.951 | 23.217 | 1.00 | 43.11 |
| ATOM | 5631 | CG | HIS | 717 | 35.745 | 7.941 | 22.112 | 1.00 | 44.69 |
| ATOM | 5632 | CD2 | HIS | 717 | 34.756 | 7.101 | 21.717 | 1.00 | 45.13 |
| ATOM | 5633 | ND1 | HIS | 717 | 36.818 | 7.683 | 21.283 | 1.00 | 47.31 |
| ATOM | 5635 | CE1 | HIS | 717 | 36.494 | 6.728 | 20.426 | 1.00 | 47.61 |
| ATOM | 5636 | NE2 | HIS | 717 | 35.250 | 6.357 | 20.670 | 1.00 | 44.95 |
| ATOM | 5638 | C | HIS | 717 | 37.451 | 7.567 | 24.413 | 1.00 | 44.84 |
| ATOM | 5639 | O | HIS | 717 | 38.528 | 8.152 | 24.295 | 1.00 | 46.79 |
| ATOM | 5640 | N | ARG | 718 | 37.313 | 6.247 | 24.337 | 1.00 | 45.44 |
| ATOM | 5642 | CA | ARG | 718 | 38.440 | 5.345 | 24.170 | 1.00 | 45.36 |
| ATOM | 5643 | CB | ARG | 718 | 38.614 | 4.496 | 25.434 | 1.00 | 43.82 |
| ATOM | 5644 | CG | ARG | 718 | 38.976 | 5.308 | 26.687 | 1.00 | 44.52 |
| ATOM | 5645 | CD | ARG | 718 | 40.284 | 6.065 | 26.476 | 1.00 | 45.02 |
| ATOM | 5646 | NE | ARG | 718 | 40.718 | 6.856 | 27.630 | 1.00 | 43.12 |
| ATOM | 5648 | CZ | ARG | 718 | 40.550 | 8.173 | 27.744 | 1.00 | 44.77 |
| ATOM | 5649 | NH1 | ARG | 718 | 39.940 | 8.859 | 26.784 | 1.00 | 44.67 |
| ATOM | 5652 | NH2 | ARG | 718 | 41.067 | 8.826 | 28.777 | 1.00 | 46.39 |
| ATOM | 5655 | C | ARG | 718 | 38.124 | 4.474 | 22.952 | 1.00 | 45.94 |
| ATOM | 5656 | O | ARG | 718 | 36.953 | 4.243 | 22.645 | 1.00 | 47.59 |
| ATOM | 5657 | N | MET | 719 | 39.145 | 4.077 | 22.204 | 1.00 | 45.34 |
| ATOM | 5659 | CA | MET | 719 | 38.925 | 3.253 | 21.029 | 1.00 | 44.28 |
| ATOM | 5660 | CB | MET | 719 | 40.198 | 3.125 | 20.185 | 1.00 | 42.30 |
| ATOM | 5661 | CG | MET | 719 | 40.575 | 4.399 | 19.441 | 1.00 | 38.44 |
| ATOM | 5662 | SD | MET | 719 | 42.000 | 4.225 | 18.368 | 1.00 | 36.97 |
| ATOM | 5663 | CE | MET | 719 | 43.317 | 4.219 | 19.511 | 1.00 | 36.09 |
| ATOM | 5664 | C | MET | 719 | 38.415 | 1.877 | 21.418 | 1.00 | 46.21 |
| ATOM | 5665 | O | MET | 719 | 38.708 | 1.393 | 22.517 | 1.00 | 43.29 |
| ATOM | 5666 | N | ASP | 720 | 37.659 | 1.267 | 20.498 | 1.00 | 48.79 |
| ATOM | 5668 | CA | ASP | 720 | 37.069 | -0.063 | 20.666 | 1.00 | 48.87 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5669 | CB | ASP | 720 | 36.099 | -0.369 | 19.513 | 1.00 | 54.01 |
| ATOM | 5670 | CG | ASP | 720 | 34.766 | 0.374 | 19.632 | 1.00 | 59.30 |
| ATOM | 5671 | OD1 | ASP | 720 | 34.762 | 1.583 | 19.981 | 1.00 | 62.96 |
| ATOM | 5672 | OD2 | ASP | 720 | 33.716 | -0.259 | 19.354 | 1.00 | 58.64 |
| ATOM | 5673 | C | ASP | 720 | 38.126 | -1.154 | 20.688 | 1.00 | 46.10 |
| ATOM | 5674 | O | ASP | 720 | 39.213 | -0.992 | 20.125 | 1.00 | 44.13 |
| ATOM | 5675 | N | LYS | 721 | 37.788 | -2.272 | 21.322 | 1.00 | 45.27 |
| ATOM | 5677 | CA | LYS | 721 | 38.689 | -3.413 | 21.404 | 1.00 | 43.25 |
| ATOM | 5678 | CB | LYS | 721 | 38.172 | -4.436 | 22.416 | 1.00 | 42.02 |
| ATOM | 5679 | CG | LYS | 721 | 39.072 | -5.651 | 22.557 | 1.00 | 46.57 |
| ATOM | 5680 | CD | LYS | 721 | 38.602 | -6.576 | 23.666 | 1.00 | 49.96 |
| ATOM | 5681 | CE | LYS | 721 | 38.300 | -7.971 | 23.141 | 1.00 | 51.80 |
| ATOM | 5682 | NZ | LYS | 721 | 37.937 | -8.920 | 24.240 | 1.00 | 56.08 |
| ATOM | 5686 | C | LYS | 721 | 38.769 | -4.055 | 20.031 | 1.00 | 43.67 |
| ATOM | 5687 | O | LYS | 721 | 37.736 | -4.313 | 19.394 | 1.00 | 44.02 |
| ATOM | 5688 | N | PRO | 722 | 39.995 | -4.233 | 19.513 | 1.00 | 43.94 |
| ATOM | 5689 | CD | PRO | 722 | 41.281 | -3.711 | 20.001 | 1.00 | 45.90 |
| ATOM | 5690 | CA | PRO | 722 | 40.159 | -4.853 | 18.198 | 1.00 | 43.96 |
| ATOM | 5691 | CB | PRO | 722 | 41.665 | -4.720 | 17.941 | 1.00 | 43.11 |
| ATOM | 5692 | CG | PRO | 722 | 42.046 | -3.509 | 18.715 | 1.00 | 45.16 |
| ATOM | 5693 | C | PRO | 722 | 39.772 | -6.317 | 18.295 | 1.00 | 43.09 |
| ATOM | 5694 | O | PRO | 722 | 39.764 | -6.888 | 19.385 | 1.00 | 41.32 |
| ATOM | 5695 | N | SER | 723 | 39.382 | -6.902 | 17.170 | 1.00 | 45.79 |
| ATOM | 5697 | CA | SER | 723 | 39.044 | -8.316 | 17.144 | 1.00 | 46.67 |
| ATOM | 5698 | CB | SER | 723 | 38.303 | -8.664 | 15.857 | 1.00 | 44.69 |
| ATOM | 5699 | OG | SER | 723 | 39.131 | -8.414 | 14.736 | 1.00 | 49.79 |
| ATOM | 5701 | C | SER | 723 | 40.422 | -8.961 | 17.148 | 1.00 | 46.90 |
| ATOM | 5702 | O | SER | 723 | 41.360 | -8.411 | 16.581 | 1.00 | 48.81 |
| ATOM | 5703 | N | ASN | 724 | 40.540 | -10.131 | 17.760 | 1.00 | 49.28 |
| ATOM | 5705 | CA | ASN | 724 | 41.826 | -10.804 | 17.849 | 1.00 | 52.10 |
| ATOM | 5706 | CB | ASN | 724 | 42.480 | -10.947 | 16.469 | 1.00 | 55.86 |
| ATOM | 5707 | CG | ASN | 724 | 41.774 | -11.957 | 15.592 | 1.00 | 58.72 |
| ATOM | 5708 | OD1 | ASN | 724 | 41.686 | -13.140 | 15.941 | 1.00 | 62.28 |
| ATOM | 5709 | ND2 | ASN | 724 | 41.258 | -11.503 | 14.449 | 1.00 | 59.56 |
| ATOM | 5712 | C | ASN | 724 | 42.665 | -9.931 | 18.770 | 1.00 | 51.97 |
| ATOM | 5713 | O | ASN | 724 | 43.621 | -9.274 | 18.369 | 1.00 | 53.85 |
| ATOM | 5714 | N | CYS | 725 | 42.202 | -9.859 | 20.004 | 1.00 | 51.02 |
| ATOM | 5716 | CA | CYS | 725 | 42.853 | -9.094 | 21.049 | 1.00 | 50.18 |
| ATOM | 5717 | CB | CYS | 725 | 42.708 | -7.583 | 20.811 | 1.00 | 47.75 |
| ATOM | 5718 | SG | CYS | 725 | 43.424 | -6.577 | 22.130 | 1.00 | 44.37 |
| ATOM | 5719 | C | CYS | 725 | 42.131 | -9.507 | 22.315 | 1.00 | 49.31 |
| ATOM | 5720 | O | CYS | 725 | 40.916 | -9.371 | 22.417 | 1.00 | 49.90 |
| ATOM | 5721 | N | THR | 726 | 42.866 | -10.088 | 23.249 | 1.00 | 48.52 |
| ATOM | 5723 | CA | THR | 726 | 42.262 | -10.541 | 24.490 | 1.00 | 49.58 |
| ATOM | 5724 | CB | THR | 726 | 43.251 | -11.444 | 25.291 | 1.00 | 49.84 |
| ATOM | 5725 | OG1 | THR | 726 | 44.236 | -10.648 | 25.976 | 1.00 | 49.05 |
| ATOM | 5727 | CG2 | THR | 726 | 43.982 | -12.363 | 24.352 | 1.00 | 47.96 |
| ATOM | 5728 | C | THR | 726 | 41.788 | -9.369 | 25.356 | 1.00 | 49.93 |
| ATOM | 5729 | O | THR | 726 | 42.305 | -8.256 | 25.244 | 1.00 | 51.55 |
| ATOM | 5730 | N | ASN | 727 | 40.829 | -9.622 | 26.242 | 1.00 | 50.48 |
| ATOM | 5732 | CA | ASN | 727 | 40.335 | -8.577 | 27.144 | 1.00 | 52.17 |
| ATOM | 5733 | CB | ASN | 727 | 39.190 | -9.099 | 28.016 | 1.00 | 57.57 |
| ATOM | 5734 | CG | ASN | 727 | 39.533 | -10.409 | 28.714 | 1.00 | 66.49 |
| ATOM | 5735 | OD1 | ASN | 727 | 40.709 | -10.786 | 28.833 | 1.00 | 70.43 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5736 | ND2 | ASN | 727 | 38.500 | -11.122 | 29.175 | 1.00 | 68.43 |
| ATOM | 5739 | C | ASN | 727 | 41.491 | -8.091 | 28.023 | 1.00 | 50.29 |
| ATOM | 5740 | O | ASN | 727 | 41.467 | -6.976 | 28.540 | 1.00 | 49.88 |
| ATOM | 5741 | N | GLU | 728 | 42.518 | -8.927 | 28.163 | 1.00 | 50.60 |
| ATOM | 5743 | CA | GLU | 728 | 43.700 | -8.597 | 28.956 | 1.00 | 49.33 |
| ATOM | 5744 | CB | GLU | 728 | 44.529 | -9.859 | 29.220 | 1.00 | 50.44 |
| ATOM | 5745 | CG | GLU | 728 | 45.802 | -9.600 | 30.008 | 1.00 | 55.30 |
| ATOM | 5746 | CD | GLU | 728 | 46.577 | -10.862 | 30.354 | 1.00 | 57.40 |
| ATOM | 5747 | OE1 | GLU | 728 | 46.716 | -11.754 | 29.489 | 1.00 | 56.75 |
| ATOM | 5748 | OE2 | GLU | 728 | 47.062 | -10.950 | 31.502 | 1.00 | 59.85 |
| ATOM | 5749 | C | GLU | 728 | 44.539 | -7.552 | 28.212 | 1.00 | 47.08 |
| ATOM | 5750 | O | GLU | 728 | 44.888 | -6.512 | 28.776 | 1.00 | 48.02 |
| ATOM | 5751 | N | LEU | 729 | 44.846 | -7.821 | 26.945 | 1.00 | 43.34 |
| ATOM | 5753 | CA | LEU | 729 | 45.630 | -6.891 | 26.129 | 1.00 | 42.01 |
| ATOM | 5754 | CB | LEU | 729 | 45.899 | -7.500 | 24.751 | 1.00 | 39.46 |
| ATOM | 5755 | CG | LEU | 729 | 46.911 | -8.639 | 24.772 | 1.00 | 40.31 |
| ATOM | 5756 | CD1 | LEU | 729 | 46.782 | -9.482 | 23.531 | 1.00 | 42.21 |
| ATOM | 5757 | CD2 | LEU | 729 | 48.314 | -8.068 | 24.900 | 1.00 | 42.49 |
| ATOM | 5758 | C | LEU | 729 | 44.901 | -5.557 | 25.980 | 1.00 | 40.61 |
| ATOM | 5759 | O | LEU | 729 | 45.510 | -4.481 | 25.953 | 1.00 | 38.33 |
| ATOM | 5760 | N | TYR | 730 | 43.580 | -5.637 | 25.909 | 1.00 | 39.07 |
| ATOM | 5762 | CA | TYR | 730 | 42.761 | -4.455 | 25.773 | 1.00 | 38.61 |
| ATOM | 5763 | CB | TYR | 730 | 41.341 | -4.837 | 25.369 | 1.00 | 36.79 |
| ATOM | 5764 | CG | TYR | 730 | 40.454 | -3.646 | 25.125 | 1.00 | 37.08 |
| ATOM | 5765 | CD1 | TYR | 730 | 40.760 | -2.721 | 24.127 | 1.00 | 32.86 |
| ATOM | 5766 | CE1 | TYR | 730 | 39.961 | -1.616 | 23.912 | 1.00 | 29.79 |
| ATOM | 5767 | CD2 | TYR | 730 | 39.328 | -3.420 | 25.916 | 1.00 | 36.99 |
| ATOM | 5768 | CE2 | TYR | 730 | 38.522 | -2.312 | 25.704 | 1.00 | 36.69 |
| ATOM | 5769 | CZ | TYR | 730 | 38.853 | -1.412 | 24.706 | 1.00 | 32.69 |
| ATOM | 5770 | OH | TYR | 730 | 38.044 | -0.320 | 24.492 | 1.00 | 38.80 |
| ATOM | 5772 | C | TYR | 730 | 42.767 | -3.662 | 27.080 | 1.00 | 39.75 |
| ATOM | 5773 | O | TYR | 730 | 42.781 | -2.430 | 27.065 | 1.00 | 40.53 |
| ATOM | 5774 | N | MET | 731 | 42.738 | -4.360 | 28.210 | 1.00 | 41.88 |
| ATOM | 5776 | CA | MET | 731 | 42.778 | -3.684 | 29.509 | 1.00 | 45.34 |
| ATOM | 5777 | CB | MET | 731 | 42.658 | -4.697 | 30.646 | 1.00 | 53.46 |
| ATOM | 5778 | CG | MET | 731 | 41.253 | -5.248 | 30.836 | 1.00 | 64.30 |
| ATOM | 5779 | SD | MET | 731 | 40.134 | -4.095 | 31.653 | 1.00 | 75.78 |
| ATOM | 5780 | CE | MET | 731 | 40.657 | -4.338 | 33.370 | 1.00 | 69.70 |
| ATOM | 5781 | C | MET | 731 | 44.099 | -2.927 | 29.614 | 1.00 | 41.53 |
| ATOM | 5782 | O | MET | 731 | 44.157 | -1.814 | 30.138 | 1.00 | 37.91 |
| ATOM | 5783 | N | MET | 732 | 45.156 | -3.545 | 29.098 | 1.00 | 40.48 |
| ATOM | 5785 | CA | MET | 732 | 46.478 | -2.937 | 29.091 | 1.00 | 40.23 |
| ATOM | 5786 | CB | MET | 732 | 47.508 | -3.872 | 28.436 | 1.00 | 40.29 |
| ATOM | 5787 | CG | MET | 732 | 48.929 | -3.307 | 28.390 | 1.00 | 38.07 |
| ATOM | 5788 | SD | MET | 732 | 50.171 | -4.522 | 27.908 | 1.00 | 37.65 |
| ATOM | 5789 | CE | MET | 732 | 50.407 | -5.343 | 29.431 | 1.00 | 37.90 |
| ATOM | 5790 | C | MET | 732 | 46.378 | -1.623 | 28.317 | 1.00 | 38.96 |
| ATOM | 5791 | O | MET | 732 | 46.843 | -0.591 | 28.790 | 1.00 | 41.36 |
| ATOM | 5792 | N | MET | 733 | 45.744 | -1.663 | 27.148 | 1.00 | 36.94 |
| ATOM | 5794 | CA | MET | 733 | 45.574 | -0.463 | 26.340 | 1.00 | 35.19 |
| ATOM | 5795 | CB | MET | 733 | 44.796 | -0.769 | 25.070 | 1.00 | 36.07 |
| ATOM | 5796 | CG | MET | 733 | 45.549 | -1.577 | 24.048 | 1.00 | 35.99 |
| ATOM | 5797 | SD | MET | 733 | 44.471 | -1.851 | 22.641 | 1.00 | 40.05 |
| ATOM | 5798 | CE | MET | 733 | 45.244 | -3.351 | 21.909 | 1.00 | 33.13 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5799 | C | MET | 733 | 44.800 | 0.560 | 27.141 | 1.00 | 37.29 |
| ATOM | 5800 | O | MET | 733 | 45.207 | 1.719 | 27.245 | 1.00 | 39.14 |
| ATOM | 5801 | N | ARG | 734 | 43.690 | 0.125 | 27.735 | 1.00 | 38.76 |
| ATOM | 5803 | CA | ARG | 734 | 42.849 | 1.014 | 28.532 | 1.00 | 39.49 |
| ATOM | 5804 | CB | ARG | 734 | 41.577 | 0.297 | 28.993 | 1.00 | 40.33 |
| ATOM | 5805 | CG | ARG | 734 | 40.699 | -0.225 | 27.856 | 1.00 | 38.02 |
| ATOM | 5806 | CD | ARG | 734 | 40.256 | 0.877 | 26.909 | 1.00 | 42.72 |
| ATOM | 5807 | NE | ARG | 734 | 39.443 | 1.898 | 27.567 | 1.00 | 48.85 |
| ATOM | 5809 | CZ | ARG | 734 | 38.120 | 1.838 | 27.700 | 1.00 | 52.35 |
| ATOM | 5810 | NH1 | ARG | 734 | 37.435 | 0.811 | 27.222 | 1.00 | 54.79 |
| ATOM | 5813 | NH2 | ARG | 734 | 37.477 | 2.804 | 28.338 | 1.00 | 54.69 |
| ATOM | 5816 | C | ARG | 734 | 43.627 | 1.587 | 29.715 | 1.00 | 38.70 |
| ATOM | 5817 | O | ARG | 734 | 43.445 | 2.757 | 30.068 | 1.00 | 40.92 |
| ATOM | 5818 | N | ASP | 735 | 44.530 | 0.782 | 30.276 | 1.00 | 38.76 |
| ATOM | 5820 | CA | ASP | 735 | 45.379 | 1.208 | 31.399 | 1.00 | 38.60 |
| ATOM | 5821 | CB | ASP | 735 | 46.325 | 0.087 | 31.825 | 1.00 | 41.34 |
| ATOM | 5822 | CG | ASP | 735 | 45.622 | -1.022 | 32.574 | 1.00 | 44.66 |
| ATOM | 5823 | OD1 | ASP | 735 | 46.048 | -2.194 | 32.428 | 1.00 | 43.15 |
| ATOM | 5824 | OD2 | ASP | 735 | 44.657 | -0.713 | 33.313 | 1.00 | 44.46 |
| ATOM | 5825 | C | ASP | 735 | 46.215 | 2.385 | 30.938 | 1.00 | 37.76 |
| ATOM | 5826 | O | ASP | 735 | 46.235 | 3.446 | 31.585 | 1.00 | 36.35 |
| ATOM | 5827 | N | CYS | 736 | 46.890 | 2.182 | 29.805 | 1.00 | 35.39 |
| ATOM | 5829 | CA | CYS | 736 | 47.730 | 3.196 | 29.181 | 1.00 | 34.77 |
| ATOM | 5830 | CB | CYS | 736 | 48.379 | 2.652 | 27.916 | 1.00 | 30.62 |
| ATOM | 5831 | SG | CYS | 736 | 49.453 | 1.261 | 28.198 | 1.00 | 30.96 |
| ATOM | 5832 | C | CYS | 736 | 46.938 | 4.429 | 28.814 | 1.00 | 35.98 |
| ATOM | 5833 | O | CYS | 736 | 47.516 | 5.491 | 28.606 | 1.00 | 37.38 |
| ATOM | 5834 | N | TRP | 737 | 45.620 | 4.290 | 28.713 | 1.00 | 38.50 |
| ATOM | 5836 | CA | TRP | 737 | 44.772 | 5.423 | 28.370 | 1.00 | 40.16 |
| ATOM | 5837 | CB | TRP | 737 | 43.791 | 5.028 | 27.271 | 1.00 | 38.41 |
| ATOM | 5838 | CG | TRP | 737 | 44.453 | 4.586 | 26.011 | 1.00 | 39.33 |
| ATOM | 5839 | CD2 | TRP | 737 | 43.893 | 3.718 | 25.020 | 1.00 | 39.64 |
| ATOM | 5840 | CE2 | TRP | 737 | 44.852 | 3.583 | 23.992 | 1.00 | 39.97 |
| ATOM | 5841 | CE3 | TRP | 737 | 42.672 | 3.040 | 24.900 | 1.00 | 37.06 |
| ATOM | 5842 | CD1 | TRP | 737 | 45.695 | 4.932 | 25.556 | 1.00 | 39.56 |
| ATOM | 5843 | NE1 | TRP | 737 | 45.941 | 4.336 | 24.343 | 1.00 | 38.61 |
| ATOM | 5845 | CZ2 | TRP | 737 | 44.627 | 2.795 | 22.859 | 1.00 | 38.78 |
| ATOM | 5846 | CZ3 | TRP | 737 | 42.452 | 2.261 | 23.778 | 1.00 | 38.90 |
| ATOM | 5847 | CH2 | TRP | 737 | 43.426 | 2.145 | 22.772 | 1.00 | 38.18 |
| ATOM | 5848 | C | TRP | 737 | 44.028 | 6.029 | 29.563 | 1.00 | 41.30 |
| ATOM | 5849 | O | TRP | 737 | 42.979 | 6.658 | 29.398 | 1.00 | 41.45 |
| ATOM | 5850 | N | HIS | 738 | 44.575 | 5.873 | 30.763 | 1.00 | 43.01 |
| ATOM | 5852 | CA | HIS | 738 | 43.932 | 6.423 | 31.948 | 1.00 | 44.64 |
| ATOM | 5853 | CB | HIS | 738 | 44.454 | 5.735 | 33.205 | 1.00 | 46.20 |
| ATOM | 5854 | CG | HIS | 738 | 43.742 | 6.154 | 34.458 | 1.00 | 50.35 |
| ATOM | 5855 | CD2 | HIS | 738 | 43.473 | 7.379 | 34.963 | 1.00 | 49.09 |
| ATOM | 5856 | ND1 | HIS | 738 | 43.220 | 5.244 | 35.355 | 1.00 | 49.94 |
| ATOM | 5858 | CE1 | HIS | 738 | 42.659 | 5.899 | 36.357 | 1.00 | 52.92 |
| ATOM | 5859 | NE2 | HIS | 738 | 42.798 | 7.194 | 36.146 | 1.00 | 46.91 |
| ATOM | 5861 | C | HIS | 738 | 44.174 | 7.921 | 32.037 | 1.00 | 45.26 |
| ATOM | 5862 | O | HIS | 738 | 45.314 | 8.356 | 32.021 | 1.00 | 45.31 |
| ATOM | 5863 | N | ALA | 739 | 43.099 | 8.686 | 32.224 | 1.00 | 46.61 |
| ATOM | 5865 | CA | ALA | 739 | 43.155 | 10.150 | 32.322 | 1.00 | 48.49 |
| ATOM | 5866 | CB | ALA | 739 | 41.823 | 10.681 | 32.790 | 1.00 | 49.69 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5867 | C | ALA | 739 | 44.272 | 10.682 | 33.224 | 1.00 | 50.77 |
| ATOM | 5868 | O | ALA | 739 | 45.004 | 11.601 | 32.846 | 1.00 | 51.77 |
| ATOM | 5869 | N | VAL | 740 | 44.336 | 10.138 | 34.439 | 1.00 | 51.47 |
| ATOM | 5871 | CA | VAL | 740 | 45.352 | 10.485 | 35.439 | 1.00 | 51.09 |
| ATOM | 5872 | CB | VAL | 740 | 44.897 | 10.075 | 36.850 | 1.00 | 52.40 |
| ATOM | 5873 | CG1 | VAL | 740 | 45.847 | 10.624 | 37.878 | 1.00 | 53.38 |
| ATOM | 5874 | CG2 | VAL | 740 | 43.485 | 10.544 | 37.105 | 1.00 | 55.18 |
| ATOM | 5875 | C | VAL | 740 | 46.649 | 9.727 | 35.130 | 1.00 | 48.99 |
| ATOM | 5876 | O | VAL | 740 | 46.773 | 8.534 | 35.440 | 1.00 | 47.72 |
| ATOM | 5877 | N | PRO | 741 | 47.646 | 10.421 | 34.565 | 1.00 | 48.31 |
| ATOM | 5878 | CD | PRO | 741 | 47.603 | 11.861 | 34.253 | 1.00 | 47.84 |
| ATOM | 5879 | CA | PRO | 741 | 48.949 | 9.852 | 34.197 | 1.00 | 48.51 |
| ATOM | 5880 | CB | PRO | 741 | 49.762 | 11.087 | 33.828 | 1.00 | 46.83 |
| ATOM | 5881 | CG | PRO | 741 | 48.714 | 12.000 | 33.255 | 1.00 | 46.21 |
| ATOM | 5882 | C | PRO | 741 | 49.641 | 9.016 | 35.275 | 1.00 | 49.12 |
| ATOM | 5883 | O | PRO | 741 | 50.449 | 8.139 | 34.955 | 1.00 | 46.57 |
| ATOM | 5884 | N | SER | 742 | 49.327 | 9.290 | 36.541 | 1.00 | 49.47 |
| ATOM | 5886 | CA | SER | 742 | 49.928 | 8.557 | 37.651 | 1.00 | 49.50 |
| ATOM | 5887 | CB | SER | 742 | 49.760 | 9.326 | 38.963 | 1.00 | 51.06 |
| ATOM | 5888 | OG | SER | 742 | 48.403 | 9.638 | 39.209 | 1.00 | 53.81 |
| ATOM | 5890 | C | SER | 742 | 49.339 | 7.159 | 37.787 | 1.00 | 48.81 |
| ATOM | 5891 | O | SER | 742 | 49.926 | 6.284 | 38.427 | 1.00 | 49.45 |
| ATOM | 5892 | N | GLN | 743 | 48.164 | 6.959 | 37.203 | 1.00 | 47.82 |
| ATOM | 5894 | CA | GLN | 743 | 47.529 | 5.658 | 37.273 | 1.00 | 46.34 |
| ATOM | 5895 | CB | GLN | 743 | 46.022 | 5.791 | 37.432 | 1.00 | 49.74 |
| ATOM | 5896 | CG | GLN | 743 | 45.519 | 5.305 | 38.784 | 1.00 | 55.41 |
| ATOM | 5897 | CD | GLN | 743 | 46.178 | 5.030 | 39.947 | 1.00 | 59.15 |
| ATOM | 5898 | OE1 | GLN | 743 | 46.905 | 5.425 | 40.748 | 1.00 | 59.02 |
| ATOM | 5899 | NE2 | GLN | 743 | 45.922 | 7.338 | 40.052 | 1.00 | 60.03 |
| ATOM | 5902 | C | GLN | 743 | 47.874 | 4.768 | 36.095 | 1.00 | 44.34 |
| ATOM | 5903 | O | GLN | 743 | 47.548 | 3.578 | 36.114 | 1.00 | 44.64 |
| ATOM | 5904 | N | ARG | 744 | 48.497 | 5.339 | 35.059 | 1.00 | 42.83 |
| ATOM | 5906 | CA | ARG | 744 | 48.914 | 4.559 | 33.880 | 1.00 | 40.34 |
| ATOM | 5907 | CB | ARG | 744 | 49.349 | 5.469 | 32.724 | 1.00 | 35.84 |
| ATOM | 5908 | CG | ARG | 744 | 48.296 | 6.406 | 32.190 | 1.00 | 28.25 |
| ATOM | 5909 | CD | ARG | 744 | 48.906 | 7.383 | 31.216 | 1.00 | 22.56 |
| ATOM | 5910 | NE | ARG | 744 | 47.948 | 8.437 | 30.922 | 1.00 | 28.09 |
| ATOM | 5912 | CZ | ARG | 744 | 48.258 | 9.658 | 30.493 | 1.00 | 32.83 |
| ATOM | 5913 | NH1 | ARG | 744 | 49.524 | 10.001 | 30.278 | 1.00 | 34.44 |
| ATOM | 5916 | NH2 | ARG | 744 | 47.307 | 10.569 | 30.360 | 1.00 | 32.00 |
| ATOM | 5919 | C | ARG | 744 | 50.110 | 3.712 | 34.295 | 1.00 | 41.58 |
| ATOM | 5920 | O | ARG | 744 | 50.906 | 4.124 | 35.145 | 1.00 | 45.48 |
| ATOM | 5921 | N | PRO | 745 | 50.223 | 2.489 | 33.754 | 1.00 | 40.97 |
| ATOM | 5922 | CD | PRO | 745 | 49.345 | 1.749 | 32.831 | 1.00 | 39.90 |
| ATOM | 5923 | CA | PRO | 745 | 51.381 | 1.685 | 34.157 | 1.00 | 39.77 |
| ATOM | 5924 | CB | PRO | 745 | 51.063 | 0.311 | 33.558 | 1.00 | 39.31 |
| ATOM | 5925 | CG | PRO | 745 | 50.255 | 0.642 | 32.344 | 1.00 | 40.98 |
| ATOM | 5926 | C | PRO | 745 | 52.664 | 2.269 | 33.573 | 1.00 | 38.44 |
| ATOM | 5927 | O | PRO | 745 | 52.631 | 3.009 | 32.595 | 1.00 | 39.64 |
| ATOM | 5928 | N | THR | 746 | 53.783 | 2.001 | 34.224 | 1.00 | 37.50 |
| ATOM | 5930 | CA | THR | 746 | 55.066 | 2.462 | 33.728 | 1.00 | 37.56 |
| ATOM | 5931 | CB | THR | 746 | 56.108 | 2.571 | 34.869 | 1.00 | 38.58 |
| ATOM | 5932 | OG1 | THR | 746 | 56.286 | 1.285 | 35.487 | 1.00 | 43.28 |
| ATOM | 5934 | CG2 | THR | 746 | 55.666 | 3.567 | 35.899 | 1.00 | 34.64 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5935 | C | THR | 746 | 55.546 | 1.393 | 32.739 | 1.00 | 36.49 |
| ATOM | 5936 | O | THR | 746 | 55.118 | 0.234 | 32.817 | 1.00 | 34.18 |
| ATOM | 5937 | N | PHE | 747 | 56.453 | 1.768 | 31.839 | 1.00 | 35.27 |
| ATOM | 5939 | CA | PHE | 747 | 56.995 | 0.814 | 30.880 | 1.00 | 33.48 |
| ATOM | 5940 | CB | PHE | 747 | 58.025 | 1.475 | 29.970 | 1.00 | 34.35 |
| ATOM | 5941 | CG | PHE | 747 | 57.419 | 2.369 | 28.920 | 1.00 | 32.49 |
| ATOM | 5942 | CD1 | PHE | 747 | 56.715 | 1.825 | 27.856 | 1.00 | 30.69 |
| ATOM | 5943 | CD2 | PHE | 747 | 57.519 | 3.749 | 29.018 | 1.00 | 32.81 |
| ATOM | 5944 | CE1 | PHE | 747 | 56.122 | 2.639 | 26.907 | 1.00 | 29.41 |
| ATOM | 5945 | CE2 | PHE | 747 | 56.926 | 4.573 | 28.072 | 1.00 | 32.93 |
| ATOM | 5946 | CZ | PHE | 747 | 56.223 | 4.014 | 27.015 | 1.00 | 31.50 |
| ATOM | 5947 | C | PHE | 747 | 57.621 | -0.363 | 31.606 | 1.00 | 34.65 |
| ATOM | 5948 | O | PHE | 747 | 57.616 | -1.474 | 31.099 | 1.00 | 36.34 |
| ATOM | 5949 | N | LYS | 748 | 58.142 | -0.128 | 32.808 | 1.00 | 37.75 |
| ATOM | 5951 | CA | LYS | 748 | 58.748 | -1.205 | 33.583 | 1.00 | 39.67 |
| ATOM | 5952 | CB | LYS | 748 | 59.382 | -0.664 | 34.873 | 1.00 | 43.06 |
| ATOM | 5953 | CG | LYS | 748 | 59.958 | -1.757 | 35.774 | 1.00 | 48.96 |
| ATOM | 5954 | CD | LYS | 748 | 60.750 | -1.207 | 36.966 | 1.00 | 52.20 |
| ATOM | 5955 | CE | LYS | 748 | 61.183 | -2.344 | 37.907 | 1.00 | 53.62 |
| ATOM | 5956 | NZ | LYS | 748 | 62.057 | -1.893 | 39.031 | 1.00 | 54.82 |
| ATOM | 5960 | C | LYS | 748 | 57.680 | -2.263 | 33.882 | 1.00 | 39.65 |
| ATOM | 5961 | O | LYS | 748 | 57.902 | -3.454 | 33.652 | 1.00 | 38.91 |
| ATOM | 5962 | N | GLN | 749 | 56.503 | -1.818 | 34.331 | 1.00 | 39.39 |
| ATOM | 5964 | CA | GLN | 749 | 55.402 | -2.742 | 34.623 | 1.00 | 40.70 |
| ATOM | 5965 | CB | GLN | 749 | 54.177 | -1.991 | 35.140 | 1.00 | 43.82 |
| ATOM | 5966 | CG | GLN | 749 | 54.395 | -1.149 | 36.373 | 1.00 | 50.97 |
| ATOM | 5967 | CD | GLN | 749 | 53.175 | -0.304 | 36.715 | 1.00 | 55.53 |
| ATOM | 5968 | OE1 | GLN | 749 | 53.272 | 0.914 | 36.895 | 1.00 | 55.80 |
| ATOM | 5969 | NE2 | GLN | 749 | 52.012 | -0.940 | 36.773 | 1.00 | 60.05 |
| ATOM | 5972 | C | GLN | 749 | 55.009 | -3.455 | 33.334 | 1.00 | 40.03 |
| ATOM | 5973 | O | GLN | 749 | 54.903 | -4.679 | 33.298 | 1.00 | 40.26 |
| ATOM | 5974 | N | LEU | 750 | 54.802 | -2.666 | 32.278 | 1.00 | 39.18 |
| ATOM | 5976 | CA | LEU | 750 | 54.400 | -3.171 | 30.964 | 1.00 | 36.65 |
| ATOM | 5977 | CB | LEU | 750 | 54.369 | -2.039 | 29.927 | 1.00 | 34.58 |
| ATOM | 5978 | CG | LEU | 750 | 53.355 | -0.910 | 30.116 | 1.00 | 32.52 |
| ATOM | 5979 | CD1 | LEU | 750 | 53.644 | 0.210 | 29.125 | 1.00 | 31.67 |
| ATOM | 5980 | CD2 | LEU | 750 | 51.947 | -1.435 | 29.935 | 1.00 | 31.37 |
| ATOM | 5981 | C | LEU | 750 | 55.321 | -4.255 | 30.477 | 1.00 | 35.81 |
| ATOM | 5982 | O | LEU | 750 | 54.856 | -5.267 | 29.963 | 1.00 | 35.81 |
| ATOM | 5983 | N | VAL | 751 | 56.626 | -4.035 | 30.620 | 1.00 | 37.38 |
| ATOM | 5985 | CA | VAL | 751 | 57.607 | -5.029 | 30.193 | 1.00 | 38.66 |
| ATOM | 5986 | CB | VAL | 751 | 59.077 | -4.545 | 30.411 | 1.00 | 35.42 |
| ATOM | 5987 | CG1 | VAL | 751 | 60.075 | -5.646 | 30.041 | 1.00 | 29.83 |
| ATOM | 5988 | CG2 | VAL | 751 | 59.342 | -3.324 | 29.559 | 1.00 | 29.95 |
| ATOM | 5989 | C | VAL | 751 | 57.337 | -6.314 | 30.974 | 1.00 | 41.63 |
| ATOM | 5990 | O | VAL | 751 | 57.312 | -7.401 | 30.396 | 1.00 | 42.43 |
| ATOM | 5991 | N | GLU | 752 | 57.051 | -6.174 | 32.267 | 1.00 | 43.35 |
| ATOM | 5993 | CA | GLU | 752 | 56.766 | -7.329 | 33.111 | 1.00 | 47.39 |
| ATOM | 5994 | CB | GLU | 752 | 56.674 | -6.914 | 34.587 | 1.00 | 50.66 |
| ATOM | 5995 | CG | GLU | 752 | 57.950 | -6.243 | 35.101 | 1.00 | 54.77 |
| ATOM | 5996 | CD | GLU | 752 | 58.006 | -6.101 | 36.612 | 1.00 | 55.14 |
| ATOM | 5997 | OE1 | GLU | 752 | 58.246 | -4.972 | 37.102 | 1.00 | 54.14 |
| ATOM | 5998 | OE2 | GLU | 752 | 57.844 | -7.131 | 37.308 | 1.00 | 57.73 |
| ATOM | 5999 | C | GLU | 752 | 55.496 | -8.068 | 32.655 | 1.00 | 46.00 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 6000 | O | GLU | 752 | 55.548 | -9.261 | 32.328 | 1.00 | 46.25 |
| ATOM | 6001 | N | ASP | 753 | 54.380 | -7.346 | 32.601 | 1.00 | 44.35 |
| ATOM | 6003 | CA | ASP | 753 | 53.099 | -7.912 | 32.180 | 1.00 | 44.19 |
| ATOM | 6004 | CB | ASP | 753 | 52.059 | -6.814 | 31.985 | 1.00 | 46.22 |
| ATOM | 6005 | CG | ASP | 753 | 51.512 | -6.279 | 33.278 | 1.00 | 50.48 |
| ATOM | 6006 | OD1 | ASP | 753 | 51.396 | -7.062 | 34.248 | 1.00 | 52.15 |
| ATOM | 6007 | OD2 | ASP | 753 | 51.170 | -5.069 | 33.306 | 1.00 | 52.20 |
| ATOM | 6008 | C | ASP | 753 | 53.244 | -8.608 | 30.849 | 1.00 | 44.54 |
| ATOM | 6009 | O | ASP | 753 | 52.770 | -9.724 | 30.674 | 1.00 | 46.03 |
| ATOM | 6010 | N | LEU | 754 | 53.880 | -7.918 | 29.906 | 1.00 | 44.43 |
| ATOM | 6012 | CA | LEU | 754 | 54.079 | -8.438 | 28.563 | 1.00 | 43.70 |
| ATOM | 6013 | CB | LEU | 754 | 54.570 | -7.339 | 27.618 | 1.00 | 43.48 |
| ATOM | 6014 | CG | LEU | 754 | 53.481 | -6.350 | 27.201 | 1.00 | 44.67 |
| ATOM | 6015 | CD1 | LEU | 754 | 54.095 | -5.218 | 26.399 | 1.00 | 44.51 |
| ATOM | 6016 | CD2 | LEU | 754 | 52.384 | -7.069 | 26.408 | 1.00 | 42.07 |
| ATOM | 6017 | C | LEU | 754 | 54.993 | -9.642 | 28.512 | 1.00 | 43.14 |
| ATOM | 6018 | O | LEU | 754 | 54.795 | -10.536 | 27.697 | 1.00 | 41.32 |
| ATOM | 6019 | N | ASP | 755 | 55.990 | -9.671 | 29.383 | 1.00 | 44.74 |
| ATOM | 6021 | CA | ASP | 755 | 56.897 | -10.800 | 29.426 | 1.00 | 47.24 |
| ATOM | 6022 | CB | ASP | 755 | 57.942 | -10.575 | 30.517 | 1.00 | 51.26 |
| ATOM | 6023 | CG | ASP | 755 | 59.121 | -11.518 | 30.407 | 1.00 | 55.39 |
| ATOM | 6024 | OD1 | ASP | 755 | 59.739 | -11.793 | 31.455 | 1.00 | 60.61 |
| ATOM | 6025 | OD2 | ASP | 755 | 59.443 | -11.970 | 29.283 | 1.00 | 57.16 |
| ATOM | 6026 | C | ASP | 755 | 56.023 | -12.005 | 29.771 | 1.00 | 47.67 |
| ATOM | 6027 | O | ASP | 755 | 56.041 | -13.032 | 29.081 | 1.00 | 45.99 |
| ATOM | 6028 | N | ARG | 756 | 55.186 | -11.816 | 30.789 | 1.00 | 46.72 |
| ATOM | 6030 | CA | ARG | 756 | 54.272 | -12.851 | 31.256 | 1.00 | 46.25 |
| ATOM | 6031 | CB | ARG | 756 | 53.519 | -12.368 | 32.499 | 1.00 | 46.31 |
| ATOM | 6032 | CG | ARG | 756 | 52.391 | -13.287 | 32.953 | 1.00 | 46.99 |
| ATOM | 6033 | CD | ARG | 756 | 51.733 | -12.776 | 34.227 | 1.00 | 48.10 |
| ATOM | 6034 | NE | ARG | 756 | 51.320 | -11.379 | 34.118 | 1.00 | 53.67 |
| ATOM | 6036 | CZ | ARG | 756 | 50.294 | -10.951 | 33.385 | 1.00 | 55.35 |
| ATOM | 6037 | NH1 | ARG | 756 | 49.562 | -11.812 | 32.684 | 1.00 | 54.10 |
| ATOM | 6040 | NH2 | ARG | 756 | 50.008 | -9.654 | 33.344 | 1.00 | 56.02 |
| ATOM | 6043 | C | ARG | 756 | 53.282 | -13.261 | 30.175 | 1.00 | 45.05 |
| ATOM | 6044 | O | ARG | 756 | 53.213 | -14.429 | 29.806 | 1.00 | 47.19 |
| ATOM | 6045 | N | ILE | 757 | 52.550 | -12.289 | 29.647 | 1.00 | 43.47 |
| ATOM | 6047 | CA | ILE | 757 | 51.552 | -12.553 | 28.617 | 1.00 | 43.80 |
| ATOM | 6048 | CB | ILE | 757 | 50.842 | -11.241 | 28.161 | 1.00 | 42.02 |
| ATOM | 6049 | CG2 | ILE | 757 | 49.811 | -11.536 | 27.086 | 1.00 | 39.63 |
| ATOM | 6050 | CG1 | ILE | 757 | 50.154 | -10.578 | 29.361 | 1.00 | 40.00 |
| ATOM | 6051 | CD1 | ILE | 757 | 49.600 | -9.212 | 29.086 | 1.00 | 42.68 |
| ATOM | 6052 | C | ILE | 757 | 52.148 | -13.296 | 27.428 | 1.00 | 46.03 |
| ATOM | 6053 | O | ILE | 757 | 51.549 | -14.250 | 26.947 | 1.00 | 47.78 |
| ATOM | 6054 | N | VAL | 758 | 53.359 | -12.925 | 27.015 | 1.00 | 49.03 |
| ATOM | 6056 | CA | VAL | 758 | 54.015 | -13.584 | 25.884 | 1.00 | 51.51 |
| ATOM | 6057 | CB | VAL | 758 | 55.412 | -12.971 | 25.556 | 1.00 | 50.75 |
| ATOM | 6058 | CG1 | VAL | 758 | 56.105 | -13.780 | 24.470 | 1.00 | 50.31 |
| ATOM | 6059 | CG2 | VAL | 758 | 55.269 | -11.541 | 25.081 | 1.00 | 52.52 |
| ATOM | 6060 | C | VAL | 758 | 54.209 | -15.050 | 26.212 | 1.00 | 54.30 |
| ATOM | 6061 | O | VAL | 758 | 53.991 | -15.915 | 25.369 | 1.00 | 54.80 |
| ATOM | 6062 | N | ALA | 759 | 54.617 | -15.311 | 27.450 | 1.00 | 57.65 |
| ATOM | 6064 | CA | ALA | 759 | 54.858 | -16.667 | 27.919 | 1.00 | 60.62 |
| ATOM | 6065 | CB | ALA | 759 | 55.423 | -16.637 | 29.327 | 1.00 | 60.32 |

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ATOM   6066  C    ALA   759     53.571  -17.478  27.889  1.00  63.25
ATOM   6067  O    ALA   759     53.568  -18.638  27.478  1.00  65.81
ATOM   6068  N    LEU   760     52.475  -16.856  28.305  1.00  63.56
ATOM   6070  CA   LEU   760     51.191  -17.533  28.333  1.00  64.25
ATOM   6071  CB   LEU   760     50.302  -16.912  29.407  1.00  65.66
ATOM   6072  CG   LEU   760     50.894  -16.962  30.820  1.00  65.62
ATOM   6073  CD1  LEU   760     49.988  -16.246  31.809  1.00  64.75
ATOM   6074  CD2  LEU   760     51.109  -18.410  31.227  1.00  66.65
ATOM   6075  C    LEU   760     50.483  -17.535  26.984  1.00  64.89
ATOM   6076  O    LEU   760     49.390  -18.088  26.860  1.00  66.37
ATOM   6077  N    THR   761     51.103  -16.933  25.973  1.00  65.24
ATOM   6079  CA   THR   761     50.516  -16.882  24.634  1.00  64.44
ATOM   6080  CB   THR   761     50.829  -15.539  23.925  1.00  62.95
ATOM   6081  OG1  THR   761     50.247  -14.463  24.669  1.00  62.70
ATOM   6083  CG2  THR   761     50.249  -15.525  22.521  1.00  60.59
ATOM   6084  C    THR   761     51.003  -18.044  23.769  1.00  64.71
ATOM   6085  O    THR   761     52.202  -18.201  23.533  1.00  64.70
ATOM   6086  SG   CYS   1603    18.536   -8.818  20.295  0.50  33.97  PRT2
ATOM   6087  CG   MET   534     69.178   12.159  22.968  0.50  31.30  PRT2
ATOM   6088  SD   MET   534     68.892   13.138  24.442  0.50  33.06  PRT2
ATOM   6089  CE   MET   534     70.060   12.456  25.568  0.50  34.22  PRT2
ATOM   6090  SG   CYS   603     56.041   -7.885  16.319  0.50  37.82  PRT2
ATOM   2682  OH2  TIP3  1       71.788   25.340   2.479  1.00  24.18
ATOM   2685  OH2  TIP3  2       40.022    4.089  16.127  1.00  43.09
ATOM   2688  OH2  TIP3  3       83.745   19.577  10.510  1.00  27.38
ATOM   2691  OH2  TIP3  4       83.420   20.163   7.482  1.00  30.85
ATOM   2694  OH2  TIP3  5       75.022   16.439   6.505  1.00  33.15
ATOM   2697  OH2  TIP3  6       86.308   19.567   9.284  1.00  33.55
ATOM   2700  OH2  TIP3  7       51.888   11.346  24.141  1.00  34.30
ATOM   2703  OH2  TIP3  8       55.125    9.616  22.499  1.00  21.44
ATOM   2706  OH2  TIP3  9       57.087    4.825  32.412  1.00  28.79
ATOM   2709  OH2  TIP3  10      52.142    4.824  13.180  1.00  21.14
ATOM   2712  OH2  TIP3  11      41.312    5.600  22.910  1.00  49.23
ATOM   2715  OH2  TIP3  12      45.083    9.130  21.671  1.00  37.09
ATOM   2718  OH2  TIP3  13      64.608   -2.335  28.803  1.00  44.31
ATOM   2721  OH2  TIP3  14      77.192   13.199  23.753  1.00  32.96
ATOM   2724  OH2  TIP3  15      79.201   17.296  17.997  1.00  38.51
ATOM   2727  OH2  TIP3  16      82.988   11.608  15.745  1.00  27.56
ATOM   2730  OH2  TIP3  17      14.096   -9.819   0.333  1.00  23.53
ATOM   2733  OH2  TIP3  18      38.325    0.249   5.313  1.00  43.17
ATOM   2736  OH2  TIP3  19      26.939    6.001   5.100  1.00  30.00
ATOM   2739  OH2  TIP3  20      34.305   -1.615  16.992  1.00  44.82
ATOM   2742  OH2  TIP3  21      20.300    2.328  27.798  1.00  45.23
ATOM   2745  OH2  TIP3  22      50.996  -11.607  38.052  1.00  43.49
ATOM   2748  OH2  TIP3  23      17.261   -6.167  -1.444  1.00  27.13
ATOM   2751  OH2  TIP3  24      27.724    8.124  14.996  1.00  31.20
ATOM   2754  OH2  TIP3  25      31.558    0.294   6.872  1.00  34.54
ATOM   2757  OH2  TIP3  26      26.907  -12.815  28.161  1.00  49.20
ATOM   2760  OH2  TIP3  27      28.705  -17.192  13.269  1.00  30.16
ATOM   2763  OH2  TIP3  28      88.639   13.953   7.692  1.00  41.04
ATOM   2766  OH2  TIP3  29      -2.328   -3.576  11.086  1.00  44.89
ATOM   2769  OH2  TIP3  30      34.919   -4.069  19.070  1.00  53.72
ATOM   2772  OH2  TIP3  31      80.124   17.865   9.324  1.00  28.96
ATOM   2775  OH2  TIP3  32       5.417    3.492  10.771  1.00  34.07
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| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2778 | OH2 | TIP3 | 33 | -10.718 | 4.889 | 11.542 | 1.00 | 30.81 |
| ATOM | 2781 | OH2 | TIP3 | 34 | 29.486 | -8.823 | 20.599 | 1.00 | 51.35 |
| ATOM | 2784 | OH2 | TIP3 | 35 | 6.151 | 3.065 | 13.821 | 1.00 | 34.56 |
| ATOM | 2787 | OH2 | TIP3 | 36 | 31.907 | 2.919 | 0.361 | 1.00 | 48.13 |
| ATOM | 2790 | OH2 | TIP3 | 37 | 19.974 | 1.928 | -3.873 | 1.00 | 30.12 |
| ATOM | 2793 | OH2 | TIP3 | 38 | 61.976 | 2.660 | 32.604 | 1.00 | 36.01 |
| ATOM | 2796 | OH2 | TIP3 | 39 | 21.084 | -7.119 | -3.759 | 1.00 | 20.12 |
| ATOM | 2799 | OH2 | TIP3 | 40 | -15.729 | 8.693 | 22.468 | 1.00 | 54.88 |
| ATOM | 2802 | OH2 | TIP3 | 41 | 40.160 | 2.461 | 8.734 | 1.00 | 37.95 |
| ATOM | 2805 | OH2 | TIP3 | 42 | 19.248 | 11.349 | 0.190 | 1.00 | 37.63 |
| ATOM | 2808 | OH2 | TIP3 | 43 | 66.856 | 9.143 | 17.185 | 1.00 | 27.91 |
| ATOM | 2811 | OH2 | TIP3 | 44 | 87.262 | 19.150 | 18.734 | 1.00 | 57.83 |
| ATOM | 2814 | OH2 | TIP3 | 45 | 74.597 | 17.144 | 3.987 | 1.00 | 42.19 |
| ATOM | 2817 | OH2 | TIP3 | 46 | 29.192 | 16.988 | 10.582 | 1.00 | 37.28 |
| ATOM | 2820 | OH2 | TIP3 | 47 | 66.415 | 7.073 | 14.829 | 1.00 | 34.86 |
| ATOM | 2823 | OH2 | TIP3 | 48 | 85.063 | 21.453 | 5.510 | 1.00 | 27.42 |
| ATOM | 2826 | OH2 | TIP3 | 49 | -4.716 | 2.835 | 2.998 | 1.00 | 40.54 |
| ATOM | 2829 | OH2 | TIP3 | 50 | 19.369 | 5.069 | 4.888 | 1.00 | 38.40 |
| ATOM | 2832 | OH2 | TIP3 | 51 | 34.750 | 5.517 | 24.999 | 1.00 | 29.11 |
| ATOM | 2835 | OH2 | TIP3 | 52 | 34.740 | -16.765 | 14.093 | 1.00 | 32.68 |
| ATOM | 2838 | OH2 | TIP3 | 53 | 59.994 | 7.555 | 27.844 | 1.00 | 32.60 |
| ATOM | 2841 | OH2 | TIP3 | 54 | -7.401 | -1.595 | 6.080 | 1.00 | 43.73 |
| ATOM | 2844 | OH2 | TIP3 | 55 | 55.257 | 12.084 | 25.108 | 1.00 | 44.32 |
| ATOM | 2847 | OH2 | TIP3 | 56 | 68.239 | 6.953 | 16.647 | 1.00 | 44.46 |
| ATOM | 2850 | OH2 | TIP3 | 57 | 73.621 | 20.852 | 18.820 | 1.00 | 29.47 |
| ATOM | 2853 | OH2 | TIP3 | 58 | 3.399 | -3.294 | -8.210 | 1.00 | 22.31 |
| ATOM | 2856 | OH2 | TIP3 | 59 | 37.999 | 10.824 | 5.505 | 1.00 | 31.62 |
| ATOM | 2859 | OH2 | TIP3 | 60 | 29.779 | -9.515 | -1.395 | 1.00 | 40.76 |
| ATOM | 2862 | OH2 | TIP3 | 61 | 49.114 | 1.432 | 12.261 | 1.00 | 29.92 |
| ATOM | 2865 | OH2 | TIP3 | 62 | 41.257 | 4.012 | 29.005 | 1.00 | 39.24 |
| ATOM | 2868 | OH2 | TIP3 | 63 | 11.113 | -12.848 | 1.296 | 1.00 | 34.36 |
| ATOM | 2871 | OH2 | TIP3 | 64 | -1.221 | -4.593 | 21.504 | 1.00 | 34.24 |
| ATOM | 2874 | OH2 | TIP3 | 65 | 30.002 | 16.453 | 13.258 | 1.00 | 49.66 |
| ATOM | 2877 | OH2 | TIP3 | 66 | 8.212 | 4.106 | 3.434 | 1.00 | 36.54 |
| ATOM | 2880 | OH2 | TIP3 | 67 | 72.868 | 18.807 | 22.589 | 1.00 | 38.26 |
| ATOM | 2883 | OH2 | TIP3 | 68 | -8.056 | -3.666 | 25.021 | 1.00 | 39.81 |
| ATOM | 2886 | OH2 | TIP3 | 69 | 66.436 | -4.683 | 28.008 | 1.00 | 60.97 |
| ATOM | 2889 | OH2 | TIP3 | 70 | 22.063 | -20.641 | 4.804 | 1.00 | 42.25 |
| ATOM | 2892 | OH2 | TIP3 | 71 | 59.860 | -7.407 | 4.859 | 1.00 | 56.78 |
| ATOM | 2895 | OH2 | TIP3 | 72 | 16.887 | -13.832 | -2.611 | 1.00 | 59.32 |
| ATOM | 2898 | OH2 | TIP3 | 73 | -15.108 | 7.351 | 4.303 | 1.00 | 31.87 |
| ATOM | 2901 | OH2 | TIP3 | 74 | 32.901 | 2.922 | 13.663 | 1.00 | 37.89 |
| ATOM | 2904 | OH2 | TIP3 | 75 | 0.173 | -2.666 | 11.035 | 1.00 | 39.12 |
| ATOM | 2907 | OH2 | TIP3 | 76 | 17.533 | 2.317 | 5.808 | 1.00 | 18.66 |
| ATOM | 2910 | OH2 | TIP3 | 77 | 27.183 | 3.730 | 6.349 | 1.00 | 29.04 |
| ATOM | 2913 | OH2 | TIP3 | 78 | -8.812 | 5.887 | 9.703 | 1.00 | 30.53 |
| ATOM | 2916 | OH2 | TIP3 | 79 | 1.614 | -2.195 | 8.694 | 1.00 | 30.79 |
| ATOM | 2919 | OH2 | TIP3 | 80 | -5.304 | -3.157 | 6.846 | 1.00 | 47.38 |
| ATOM | 2922 | OH2 | TIP3 | 81 | 17.401 | 2.918 | 1.973 | 1.00 | 20.47 |
| ATOM | 2925 | OH2 | TIP3 | 82 | 20.333 | 3.188 | 3.159 | 1.00 | 24.44 |
| ATOM | 2928 | OH2 | TIP3 | 83 | 0.408 | -2.516 | 22.276 | 1.00 | 31.11 |
| ATOM | 2931 | OH2 | TIP3 | 84 | 20.095 | -6.123 | -1.372 | 1.00 | 17.62 |
| ATOM | 2934 | OH2 | TIP3 | 85 | 11.018 | -15.627 | 7.421 | 1.00 | 60.29 |
| ATOM | 2937 | OH2 | TIP3 | 86 | 4.089 | -12.037 | 11.797 | 1.00 | 39.47 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2940 | OH2 | TIP3 | 87 | 6.459 | 0.908 | -3.278 | 1.00 | 30.31 |
| ATOM | 2943 | OH2 | TIP3 | 88 | -13.493 | 1.004 | 5.319 | 1.00 | 41.13 |
| ATOM | 2946 | OH2 | TIP3 | 89 | 15.418 | -7.532 | 0.022 | 1.00 | 21.29 |
| ATOM | 2949 | OH2 | TIP3 | 90 | -2.128 | -5.834 | 4.052 | 1.00 | 57.55 |
| ATOM | 2952 | OH2 | TIP3 | 91 | 12.731 | 4.833 | -4.212 | 1.00 | 44.52 |
| ATOM | 2955 | OH2 | TIP3 | 92 | 69.320 | 27.812 | 2.191 | 1.00 | 37.47 |
| ATOM | 2958 | OH2 | TIP3 | 93 | 24.851 | -12.871 | 0.285 | 1.00 | 44.73 |
| ATOM | 2961 | OH2 | TIP3 | 94 | 60.301 | -4.459 | 33.927 | 1.00 | 40.13 |
| ATOM | 2964 | OH2 | TIP3 | 95 | 10.488 | 5.951 | 3.205 | 1.00 | 41.53 |
| ATOM | 2967 | OH2 | TIP3 | 96 | -9.708 | -4.233 | 4.439 | 1.00 | 29.77 |
| ATOM | 2970 | OH2 | TIP3 | 97 | 72.950 | -1.768 | 10.144 | 1.00 | 39.69 |
| ATOM | 2973 | OH2 | TIP3 | 98 | -3.287 | 5.612 | 30.618 | 1.00 | 34.65 |
| ATOM | 2976 | OH2 | TIP3 | 99 | 36.658 | 1.007 | 11.717 | 1.00 | 35.43 |
| ATOM | 2979 | OH2 | TIP3 | 100 | 21.221 | 6.459 | 16.863 | 1.00 | 20.70 |
| ATOM | 2982 | OH2 | TIP3 | 101 | 5.833 | -8.726 | 22.274 | 1.00 | 47.13 |
| ATOM | 2985 | OH2 | TIP3 | 102 | -13.529 | 7.868 | 17.445 | 1.00 | 31.95 |
| ATOM | 2988 | OH2 | TIP3 | 103 | 26.795 | -10.682 | -0.807 | 1.00 | 28.65 |
| ATOM | 2991 | OH2 | TIP3 | 104 | 23.711 | 1.909 | 18.309 | 1.00 | 28.29 |
| ATOM | 2994 | OH2 | TIP3 | 105 | -2.187 | 12.232 | 3.920 | 1.00 | 44.98 |
| ATOM | 2997 | OH2 | TIP3 | 106 | 59.483 | 12.398 | 33.535 | 1.00 | 39.58 |
| ATOM | 3000 | OH2 | TIP3 | 107 | 4.439 | -10.915 | 1.996 | 1.00 | 43.77 |
| ATOM | 3003 | OH2 | TIP3 | 108 | 8.041 | 2.687 | 0.648 | 1.00 | 45.32 |
| ATOM | 3006 | OH2 | TIP3 | 109 | 75.836 | 1.477 | 25.476 | 1.00 | 41.65 |
| ATOM | 3009 | OH2 | TIP3 | 110 | 48.604 | 15.594 | 14.349 | 1.00 | 36.36 |
| ATOM | 3012 | OH2 | TIP3 | 111 | 2.396 | -11.387 | 9.259 | 1.00 | 34.21 |
| ATOM | 3015 | OH2 | TIP3 | 112 | 82.927 | 26.453 | 12.807 | 1.00 | 36.54 |
| ATOM | 3018 | OH2 | TIP3 | 113 | 8.983 | -6.631 | -3.299 | 1.00 | 47.01 |
| ATOM | 3021 | OH2 | TIP3 | 114 | -8.690 | 4.367 | 4.504 | 1.00 | 41.25 |
| ATOM | 3024 | OH2 | TIP3 | 115 | 7.941 | -13.921 | 8.777 | 1.00 | 36.12 |
| ATOM | 3027 | OH2 | TIP3 | 116 | 51.295 | 6.440 | 10.632 | 1.00 | 28.37 |
| ATOM | 3030 | OH2 | TIP3 | 117 | 20.432 | 3.771 | 15.637 | 1.00 | 31.22 |
| ATOM | 3033 | OH2 | TIP3 | 118 | 72.882 | 3.887 | 20.227 | 1.00 | 30.22 |
| ATOM | 3036 | OH2 | TIP3 | 119 | 5.187 | -11.863 | 22.711 | 1.00 | 47.49 |
| ATOM | 3039 | OH2 | TIP3 | 120 | 33.889 | 2.571 | 16.293 | 1.00 | 40.04 |
| ATOM | 3042 | OH2 | TIP3 | 121 | 9.504 | -12.183 | 7.160 | 1.00 | 31.48 |
| ATOM | 3045 | OH2 | TIP3 | 122 | 8.397 | 3.827 | -1.647 | 1.00 | 46.92 |
| ATOM | 3048 | OH2 | TIP3 | 123 | 7.281 | 7.321 | 2.391 | 1.00 | 62.46 |
| ATOM | 3051 | OH2 | TIP3 | 124 | 35.682 | -1.725 | 0.534 | 1.00 | 36.75 |
| ATOM | 3054 | OH2 | TIP3 | 125 | 44.465 | 10.095 | 11.089 | 1.00 | 44.72 |
| ATOM | 3057 | OH2 | TIP3 | 126 | 45.247 | 11.893 | 21.405 | 1.00 | 33.51 |
| ATOM | 3060 | OH2 | TIP3 | 127 | 57.386 | -10.506 | 14.020 | 1.00 | 45.72 |
| ATOM | 3063 | OH2 | TIP3 | 128 | -3.033 | 15.103 | 16.644 | 1.00 | 38.48 |
| ATOM | 3066 | OH2 | TIP3 | 129 | 85.621 | 11.111 | 8.814 | 1.00 | 38.13 |
| ATOM | 3069 | OH2 | TIP3 | 130 | 13.040 | -2.760 | 2.176 | 1.00 | 31.26 |
| ATOM | 3072 | OH2 | TIP3 | 131 | 75.607 | 3.932 | 20.836 | 1.00 | 55.09 |
| ATOM | 3075 | OH2 | TIP3 | 132 | 13.080 | 7.467 | -2.358 | 1.00 | 35.05 |
| ATOM | 3078 | OH2 | TIP3 | 133 | 11.308 | -9.967 | 0.995 | 1.00 | 28.96 |
| ATOM | 3081 | OH2 | TIP3 | 134 | 13.716 | -16.170 | 3.848 | 1.00 | 44.64 |
| ATOM | 3084 | OH2 | TIP3 | 135 | -6.498 | -3.706 | 16.178 | 1.00 | 43.17 |
| ATOM | 3087 | OH2 | TIP3 | 136 | 25.841 | -12.949 | 3.950 | 1.00 | 41.14 |
| ATOM | 3090 | OH2 | TIP3 | 137 | -16.285 | 10.803 | 6.585 | 1.00 | 45.75 |
| ATOM | 3093 | OH2 | TIP3 | 138 | 86.457 | 12.585 | 6.477 | 1.00 | 36.37 |
| ATOM | 3096 | OH2 | TIP3 | 139 | 32.097 | -4.644 | 2.224 | 1.00 | 28.35 |
| ATOM | 3099 | OH2 | TIP3 | 140 | 44.936 | 7.528 | 11.961 | 1.00 | 46.60 |

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ATOM   3102  OH2  TIP3 141      80.781    12.162    16.353   1.00    41.46
ATOM   3105  OH2  TIP3 142       2.547    -7.532    -1.453   1.00    41.42
ATOM   3108  OH2  TIP3 143      31.850    -5.907    21.194   1.00    54.70
ATOM   3111  OH2  TIP3 144      74.524    -2.663    12.264   1.00    40.35
ATOM   3114  OH2  TIP3 145       7.592     6.769    -0.931   1.00    58.34
ATOM   3117  OH2  TIP3 146      71.168     5.735    21.648   1.00    27.86
ATOM   3120  OH2  TIP3 147      67.876    -4.900     8.725   1.00    33.58
ATOM   3123  OH2  TIP3 148       0.554   -10.181     6.605   1.00    75.65
ATOM   3126  OH2  TIP3 149      67.965    18.266    10.874   1.00    30.42
ATOM   3129  OH2  TIP3 150       3.509     8.125     4.021   1.00    40.77
ATOM   3132  OH2  TIP3 151      52.216    12.175    18.131   1.00    47.63
ATOM   3135  OH2  TIP3 152     -10.336     6.394     5.014   1.00    48.53
ATOM   3138  OH2  TIP3 153      76.427     1.384    -1.196   1.00    47.21
ATOM   3141  OH2  TIP3 154      10.116   -12.199    17.089   1.00    70.16
ATOM   3144  OH2  TIP3 155      34.043    14.595    18.314   1.00    40.56
ATOM   3147  OH2  TIP3 156       2.488    -8.304    16.835   1.00    64.47
ATOM   3150  OH2  TIP3 157      29.610     1.954     6.685   1.00    48.74
ATOM   3153  OH2  TIP3 158      32.578   -17.270    12.109   1.00    37.35
ATOM   3156  OH2  TIP3 159      42.013    18.106    11.196   1.00    68.33
ATOM   3159  OH2  TIP3 160      87.646    10.346     5.465   1.00    75.39
ATOM   3162  OH2  TIP3 161      69.931    -3.739    24.921   1.00    70.42
ATOM   3165  OH2  TIP3 162      77.277     5.700    23.531   1.00    53.26
ATOM   3168  OH2  TIP3 163      34.172    15.704     1.865   1.00    44.88
ATOM   3171  OH2  TIP3 164      -9.871     7.514     7.751   1.00    39.18
ATOM   3174  OH2  TIP3 165      11.814     5.604     7.443   1.00    46.70
ATOM   3177  OH2  TIP3 166      -8.801    13.912    13.532   1.00    52.89
ATOM   3180  OH2  TIP3 167      32.195     3.409    18.336   1.00    32.33
ATOM   3183  OH2  TIP3 168      -8.858     9.696    24.279   1.00    38.90
ATOM   3186  OH2  TIP3 169      -1.135    -6.924    15.691   1.00    43.05
ATOM   3189  OH2  TIP3 170      79.806     0.323    15.371   1.00    36.91
ATOM   3192  OH2  TIP3 171      67.181    20.622    -1.545   1.00    44.72
ATOM   3195  OH2  TIP3 172      -0.823     3.732     1.065   1.00    52.11
ATOM   3198  OH2  TIP3 173      -0.130     6.021     2.491   1.00    40.87
ATOM   3201  OH2  TIP3 174      -1.027     8.941     1.064   1.00    60.72
ATOM   3204  OH2  TIP3 175      -5.566     8.867     2.163   1.00    47.25
ATOM   3207  OH2  TIP3 176      -7.259    10.294     4.033   1.00    53.61
ATOM   3210  OH2  TIP3 177       2.664     7.247     1.058   1.00    46.41
ATOM   3213  OH2  TIP3 178       5.295    10.728     8.257   1.00    39.84
ATOM   3216  OH2  TIP3 179      63.743    12.726    22.713   1.00    49.55
ATOM   3219  OH2  TIP3 180      79.165     1.016    17.948   1.00    51.41
ATOM   3222  OH2  TIP3 181      13.823    -1.538    -3.942   1.00    39.85
ATOM   3225  OH2  TIP3 182      59.255     3.213    32.873   1.00    76.77
ATOM   3228  OH2  TIP3 183      32.210    13.612    20.027   1.00    60.41
ATOM   3231  OH2  TIP3 184      72.606    16.267    22.574   1.00    60.78
ATOM   3234  OH2  TIP3 185      -0.147     5.713    30.877   1.00    50.19
ATOM   3237  OH2  TIP3 186      -1.207    -4.507    27.969   1.00    65.19
ATOM   3240  OH2  TIP3 187      81.340    15.584    16.808   1.00    64.48
ATOM   3243  OH2  TIP3 188     -17.535     3.884    23.785   1.00    57.17
ATOM   3246  OH2  TIP3 189      27.503    10.697    14.669   1.00    36.11
ATOM   3249  OH2  TIP3 190      34.585     4.535    27.618   1.00    61.68
ATOM   3252  OH2  TIP3 191      -3.701    -4.982     9.069   1.00    43.66
ATOM   3255  OH2  TIP3 192      42.524     7.811    22.390   1.00    34.53
ATOM   3258  OH2  TIP3 193      52.937    11.764    21.790   1.00    36.19
ATOM   3261  OH2  TIP3 194      -7.665     8.600     6.358   1.00    59.08
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3264 | OH2 | TIP3 | 195 | 86.880 | 5.187 | 16.579 | 1.00 | 55.88 |
| ATOM | 3267 | OH2 | TIP3 | 196 | 55.377 | 16.147 | 20.540 | 1.00 | 48.25 |
| ATOM | 3270 | OH2 | TIP3 | 197 | 51.394 | 19.664 | 22.988 | 1.00 | 46.81 |
| ATOM | 3273 | OH2 | TIP3 | 198 | 20.021 | 7.087 | 7.226 | 1.00 | 52.98 |
| ATOM | 3276 | OH2 | TIP3 | 199 | 28.959 | 1.819 | -3.219 | 1.00 | 40.50 |
| ATOM | 3279 | OH2 | TIP3 | 200 | 26.533 | 2.812 | -4.295 | 1.00 | 54.24 |
| ATOM | 3282 | OH2 | TIP3 | 201 | 36.739 | 3.003 | 18.397 | 1.00 | 42.13 |
| ATOM | 3285 | OH2 | TIP3 | 202 | 16.968 | -20.752 | 14.318 | 1.00 | 54.54 |
| ATOM | 3288 | OH2 | TIP3 | 203 | 28.177 | -14.418 | 6.134 | 1.00 | 61.36 |
| ATOM | 3291 | OH2 | TIP3 | 204 | 31.488 | 1.501 | -1.796 | 1.00 | 47.49 |
| ATOM | 3294 | OH2 | TIP3 | 205 | 10.665 | -16.494 | 15.731 | 1.00 | 41.42 |
| ATOM | 3297 | OH2 | TIP3 | 206 | 6.916 | -12.200 | 6.160 | 1.00 | 61.94 |
| ATOM | 3300 | OH2 | TIP3 | 207 | -12.659 | 14.357 | 10.908 | 1.00 | 52.96 |
| ATOM | 3303 | OH2 | TIP3 | 208 | 11.274 | 9.662 | -1.588 | 1.00 | 48.45 |
| ATOM | 3306 | OH2 | TIP3 | 209 | 11.491 | 12.484 | -1.531 | 1.00 | 44.51 |
| ATOM | 3309 | OH2 | TIP3 | 210 | 34.037 | 13.520 | -1.011 | 1.00 | 48.43 |
| ATOM | 3312 | OH2 | TIP3 | 211 | 31.162 | 18.259 | 7.980 | 1.00 | 44.86 |
| ATOM | 3315 | OH2 | TIP3 | 212 | 36.937 | 11.633 | -1.971 | 1.00 | 49.85 |
| ATOM | 3318 | OH2 | TIP3 | 213 | 64.024 | 13.599 | 26.505 | 1.00 | 37.53 |
| ATOM | 3321 | OH2 | TIP3 | 214 | 36.528 | 5.933 | 14.857 | 1.00 | 57.04 |
| ATOM | 3324 | OH2 | TIP3 | 215 | 90.599 | 4.042 | 6.342 | 1.00 | 54.08 |
| ATOM | 3327 | OH2 | TIP3 | 216 | 50.139 | -11.645 | 10.526 | 1.00 | 54.64 |
| ATOM | 3330 | OH2 | TIP3 | 217 | 66.523 | -1.024 | 30.536 | 1.00 | 39.41 |
| ATOM | 3333 | OH2 | TIP3 | 218 | 74.880 | 18.976 | 20.591 | 1.00 | 41.84 |
| ATOM | 3336 | OH2 | TIP3 | 219 | -3.095 | 9.744 | 3.142 | 1.00 | 52.35 |
| ATOM | 3339 | OH2 | TIP3 | 220 | 5.601 | -3.682 | 25.022 | 1.00 | 29.30 |
| ATOM | 3342 | OH2 | TIP3 | 221 | 35.616 | 6.407 | 12.455 | 1.00 | 44.48 |
| ATOM | 3345 | OH2 | TIP3 | 222 | -5.381 | 16.006 | 14.081 | 1.00 | 44.23 |
| ATOM | 3348 | OH2 | TIP3 | 223 | 46.509 | -11.503 | 26.814 | 1.00 | 53.82 |
| ATOM | 3351 | OH2 | TIP3 | 224 | -3.791 | -5.481 | 20.929 | 1.00 | 61.42 |
| ATOM | 3354 | OH2 | TIP3 | 225 | 1.622 | -3.876 | -0.402 | 1.00 | 58.60 |
| ATOM | 3357 | OH2 | TIP3 | 226 | 86.244 | 11.220 | 23.133 | 1.00 | 59.84 |
| ATOM | 3360 | OH2 | TIP3 | 227 | 11.011 | 7.959 | 5.659 | 1.00 | 63.07 |
| ATOM | 3363 | OH2 | TIP3 | 228 | 64.610 | -8.031 | 20.406 | 1.00 | 48.11 |
| ATOM | 3366 | OH2 | TIP3 | 229 | 11.446 | -17.829 | 13.438 | 1.00 | 51.35 |
| ATOM | 3369 | OH2 | TIP3 | 230 | 72.056 | 1.258 | -1.830 | 1.00 | 43.88 |
| ATOM | 3372 | OH2 | TIP3 | 231 | 57.359 | 9.732 | 11.744 | 1.00 | 65.45 |
| ATOM | 3375 | OH2 | TIP3 | 232 | 43.344 | 20.728 | 30.066 | 1.00 | 61.52 |
| ATOM | 3378 | OH2 | TIP3 | 233 | 66.723 | 16.772 | 15.661 | 1.00 | 43.79 |
| ATOM | 3381 | OH2 | TIP3 | 234 | 88.036 | 22.036 | 4.257 | 1.00 | 61.83 |
| ATOM | 3384 | OH2 | TIP3 | 235 | 12.085 | 2.346 | 27.862 | 1.00 | 46.29 |
| ATOM | 3387 | OH2 | TIP3 | 236 | 64.898 | -0.425 | 3.209 | 1.00 | 50.06 |
| ATOM | 3390 | OH2 | TIP3 | 237 | 72.114 | 28.348 | 7.731 | 1.00 | 53.01 |
| ATOM | 3393 | OH2 | TIP3 | 238 | 25.792 | -8.081 | 27.181 | 1.00 | 55.19 |
| ATOM | 3396 | OH2 | TIP3 | 239 | -18.262 | 10.614 | 12.607 | 1.00 | 51.54 |
| ATOM | 3399 | OH2 | TIP3 | 240 | 30.336 | 11.280 | 16.201 | 1.00 | 46.53 |
| ATOM | 3402 | OH2 | TIP3 | 241 | 22.712 | -15.818 | -2.226 | 1.00 | 47.29 |
| ATOM | 3405 | OH2 | TIP3 | 242 | 29.700 | 9.496 | 18.074 | 1.00 | 40.10 |
| ATOM | 3408 | OH2 | TIP3 | 243 | 63.297 | -0.480 | 5.497 | 1.00 | 49.90 |
| ATOM | 3411 | OH2 | TIP3 | 244 | 61.458 | 7.093 | 11.497 | 1.00 | 45.71 |
| ATOM | 3414 | OH2 | TIP3 | 245 | -0.217 | 2.232 | 32.172 | 1.00 | 46.12 |
| ATOM | 3417 | OH2 | TIP3 | 246 | 66.196 | 6.250 | 12.159 | 1.00 | 34.47 |

## TABLE 3

| | Atom No. | Atom Type | A.A Type | A.A No. | X | Y | Z | OCC | B |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1 | N | GLU | 1464 | -13.712 | 16.996 | 8.424 | 1.00 | 61.15 |
| ATOM | 3 | CA | GLU | 1464 | -12.478 | 17.133 | 7.646 | 1.00 | 60.03 |
| ATOM | 4 | CB | GLU | 1464 | -11.465 | 18.020 | 8.378 | 1.00 | 62.43 |
| ATOM | 5 | C | GLU | 1464 | -11.865 | 15.766 | 7.319 | 1.00 | 57.36 |
| ATOM | 6 | O | GLU | 1464 | -11.765 | 15.402 | 6.145 | 1.00 | 60.80 |
| ATOM | 7 | N | LEU | 1465 | -11.466 | 15.003 | 8.333 | 1.00 | 50.25 |
| ATOM | 9 | CA | LEU | 1465 | -10.899 | 13.691 | 8.067 | 1.00 | 42.73 |
| ATOM | 10 | CB | LEU | 1465 | -10.097 | 13.171 | 9.258 | 1.00 | 41.34 |
| ATOM | 11 | CG | LEU | 1465 | -8.571 | 13.277 | 9.169 | 1.00 | 39.78 |
| ATOM | 12 | CD1 | LEU | 1465 | -8.175 | 14.728 | 8.977 | 1.00 | 45.14 |
| ATOM | 13 | CD2 | LEU | 1465 | -7.926 | 12.722 | 10.426 | 1.00 | 34.20 |
| ATOM | 14 | C | LEU | 1465 | -12.009 | 12.706 | 7.748 | 1.00 | 39.42 |
| ATOM | 15 | O | LEU | 1465 | -13.070 | 12.719 | 8.375 | 1.00 | 36.63 |
| ATOM | 16 | N | PRO | 1466 | -11.821 | 11.919 | 6.682 | 1.00 | 38.54 |
| ATOM | 17 | CD | PRO | 1466 | -10.682 | 12.019 | 5.751 | 1.00 | 37.04 |
| ATOM | 18 | CA | PRO | 1466 | -12.781 | 10.902 | 6.232 | 1.00 | 38.75 |
| ATOM | 19 | CB | PRO | 1466 | -12.176 | 10.426 | 4.910 | 1.00 | 39.49 |
| ATOM | 20 | CG | PRO | 1466 | -10.681 | 10.667 | 5.109 | 1.00 | 40.64 |
| ATOM | 21 | C | PRO | 1466 | -12.859 | 9.756 | 7.246 | 1.00 | 39.08 |
| ATOM | 22 | O | PRO | 1466 | -11.834 | 9.283 | 7.748 | 1.00 | 41.23 |
| ATOM | 23 | N | GLU | 1467 | -14.064 | 9.278 | 7.513 | 1.00 | 37.11 |
| ATOM | 25 | CA | GLU | 1467 | -14.247 | 8.213 | 8.482 | 1.00 | 35.96 |
| ATOM | 26 | CB | GLU | 1467 | -15.725 | 8.123 | 8.863 | 1.00 | 39.90 |
| ATOM | 27 | CG | GLU | 1467 | -16.334 | 9.410 | 9.417 | 1.00 | 46.64 |
| ATOM | 28 | CD | GLU | 1467 | -17.823 | 9.280 | 9.694 | 1.00 | 51.50 |
| ATOM | 29 | OE1 | GLU | 1467 | -18.294 | 8.135 | 9.854 | 1.00 | 54.17 |
| ATOM | 30 | OE2 | GLU | 1467 | -18.529 | 10.315 | 9.756 | 1.00 | 53.39 |
| ATOM | 31 | C | GLU | 1467 | -13.794 | 6.865 | 7.939 | 1.00 | 33.77 |
| ATOM | 32 | O | GLU | 1467 | -13.885 | 6.632 | 6.740 | 1.00 | 36.27 |
| ATOM | 33 | N | ASP | 1468 | -13.291 | 5.991 | 8.813 | 1.00 | 29.80 |
| ATOM | 35 | CA | ASP | 1468 | -12.869 | 4.649 | 8.409 | 1.00 | 28.19 |
| ATOM | 36 | CB | ASP | 1468 | -11.362 | 4.567 | 8.120 | 1.00 | 27.83 |
| ATOM | 37 | CG | ASP | 1468 | -10.942 | 3.223 | 7.507 | 1.00 | 27.78 |
| ATOM | 38 | OD1 | ASP | 1468 | -11.689 | 2.225 | 7.592 | 1.00 | 25.64 |
| ATOM | 39 | OD2 | ASP | 1468 | -9.836 | 3.165 | 6.935 | 1.00 | 27.59 |
| ATOM | 40 | C | ASP | 1468 | -13.244 | 3.672 | 9.512 | 1.00 | 28.05 |
| ATOM | 41 | O | ASP | 1468 | -12.462 | 3.404 | 10.437 | 1.00 | 25.89 |
| ATOM | 42 | N | PRO | 1469 | -14.446 | 3.089 | 9.403 | 1.00 | 29.07 |
| ATOM | 43 | CD | PRO | 1469 | -15.401 | 3.311 | 8.298 | 1.00 | 29.93 |
| ATOM | 44 | CA | PRO | 1469 | -14.981 | 2.124 | 10.365 | 1.00 | 28.65 |
| ATOM | 45 | CB | PRO | 1469 | -16.235 | 1.615 | 9.659 | 1.00 | 30.89 |
| ATOM | 46 | CG | PRO | 1469 | -16.690 | 2.811 | 8.879 | 1.00 | 28.99 |
| ATOM | 47 | C | PRO | 1469 | -14.029 | 0.974 | 10.687 | 1.00 | 27.63 |
| ATOM | 48 | O | PRO | 1469 | -14.136 | 0.364 | 11.748 | 1.00 | 26.94 |
| ATOM | 49 | N | ARG | 1470 | -13.128 | 0.666 | 9.758 | 1.00 | 26.37 |
| ATOM | 51 | CA | ARG | 1470 | -12.161 | -0.414 | 9.947 | 1.00 | 26.64 |

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ATOM     52  CB   ARG  1470     -11.363   -0.661    8.666   1.00  27.12
ATOM     53  CG   ARG  1470     -12.150   -1.014    7.424   1.00  29.72
ATOM     54  CD   ARG  1470     -11.189   -1.184    6.236   1.00  30.37
ATOM     55  NE   ARG  1470     -10.450    0.044    5.971   1.00  32.56
ATOM     57  CZ   ARG  1470      -9.624    0.211    4.948   1.00  37.69
ATOM     58  NH1  ARG  1470      -9.428   -0.784    4.091   1.00  44.25
ATOM     61  NH2  ARG  1470      -8.997    1.370    4.778   1.00  34.12
ATOM     64  C    ARG  1470     -11.129   -0.176   11.051   1.00  27.58
ATOM     65  O    ARG  1470     -10.504   -1.123   11.522   1.00  28.12
ATOM     66  N    TRP  1471     -10.900    1.079   11.421   1.00  27.62
ATOM     68  CA   TRP  1471      -9.870    1.362   12.408   1.00  26.66
ATOM     69  CB   TRP  1471      -8.661    1.938   11.686   1.00  24.95
ATOM     70  CG   TRP  1471      -8.010    0.951   10.790   1.00  25.65
ATOM     71  CD2  TRP  1471      -7.100   -0.083   11.186   1.00  23.19
ATOM     72  CE2  TRP  1471      -6.734   -0.776   10.022   1.00  21.80
ATOM     73  CE3  TRP  1471      -6.567   -0.489   12.414   1.00  21.84
ATOM     74  CD1  TRP  1471      -8.155    0.843    9.435   1.00  23.15
ATOM     75  NE1  TRP  1471      -7.388   -0.192    8.970   1.00  23.32
ATOM     77  CZ2  TRP  1471      -5.855   -1.857   10.052   1.00  22.54
ATOM     78  CZ3  TRP  1471      -5.698   -1.564   12.439   1.00  21.72
ATOM     79  CH2  TRP  1471      -5.352   -2.235   11.269   1.00  21.90
ATOM     80  C    TRP  1471     -10.224    2.278   13.558   1.00  28.44
ATOM     81  O    TRP  1471      -9.497    2.334   14.546   1.00  29.29
ATOM     82  N    GLU  1472     -11.317    3.015   13.424   1.00  29.49
ATOM     84  CA   GLU  1472     -11.719    3.962   14.453   1.00  29.97
ATOM     85  CB   GLU  1472     -12.920    4.769   13.961   1.00  33.80
ATOM     86  CG   GLU  1472     -13.218    6.050   14.731   1.00  33.27
ATOM     87  CD   GLU  1472     -12.475    7.249   14.195   1.00  34.26
ATOM     88  OE1  GLU  1472     -11.970    7.191   13.055   1.00  38.00
ATOM     89  OE2  GLU  1472     -12.413    8.265   14.910   1.00  34.01
ATOM     90  C    GLU  1472     -12.034    3.366   15.826   1.00  27.30
ATOM     91  O    GLU  1472     -12.640    2.309   15.945   1.00  28.36
ATOM     92  N    LEU  1473     -11.619    4.069   16.866   1.00  25.91
ATOM     94  CA   LEU  1473     -11.896    3.652   18.229   1.00  24.89
ATOM     95  CB   LEU  1473     -10.625    3.210   18.948   1.00  24.70
ATOM     96  CG   LEU  1473     -10.766    2.923   20.454   1.00  24.56
ATOM     97  CD1  LEU  1473     -11.498    1.613   20.701   1.00  21.89
ATOM     98  CD2  LEU  1473      -9.385    2.872   21.095   1.00  23.90
ATOM     99  C    LEU  1473     -12.426    4.907   18.882   1.00  27.05
ATOM    100  O    LEU  1473     -11.968    6.016   18.567   1.00  25.17
ATOM    101  N    PRO  1474     -13.479    4.766   19.706   1.00  28.20
ATOM    102  CD   PRO  1474     -14.290    3.551   19.886   1.00  29.92
ATOM    103  CA   PRO  1474     -14.088    5.897   20.411   1.00  30.61
ATOM    104  CB   PRO  1474     -15.197    5.224   21.226   1.00  28.15
ATOM    105  CG   PRO  1474     -15.613    4.110   20.357   1.00  24.28
ATOM    106  C    PRO  1474     -13.036    6.545   21.312   1.00  32.98
ATOM    107  O    PRO  1474     -12.253    5.838   21.968   1.00  34.79
ATOM    108  N    ARG  1475     -13.035    7.875   21.366   1.00  32.75
ATOM    110  CA   ARG  1475     -12.060    8.606   22.168   1.00  34.22
ATOM    111  CB   ARG  1475     -12.250   10.116   21.997   1.00  34.21
ATOM    112  CG   ARG  1475     -12.153   10.549   20.559   1.00  42.48
ATOM    113  CD   ARG  1475     -11.956   12.056   20.364   1.00  45.16
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ATOM   114  NE  ARG  1475      -11.655  12.317  18.954  1.00 45.65
ATOM   116  CZ  ARG  1475      -10.447  12.599  18.484  1.00 41.31
ATOM   117  NH1 ARG  1475       -9.420  12.686  19.318  1.00 35.94
ATOM   120  NH2 ARG  1475      -10.253  12.673  17.172  1.00 42.37
ATOM   123  C   ARG  1475      -12.114   8.232  23.641  1.00 35.29
ATOM   124  O   ARG  1475      -11.094   8.178  24.318  1.00 37.28
ATOM   125  N   ASP  1476      -13.304   7.931  24.129  1.00 35.37
ATOM   127  CA  ASP  1476      -13.468   7.570  25.526  1.00 36.97
ATOM   128  CB  ASP  1476      -14.952   7.586  25.896  1.00 39.47
ATOM   129  CG  ASP  1476      -15.748   6.501  25.205  1.00 40.02
ATOM   130  OD1 ASP  1476      -15.221   5.809  24.320  1.00 41.08
ATOM   131  OD2 ASP  1476      -16.926   6.327  25.571  1.00 47.00
ATOM   132  C   ASP  1476      -12.850   6.225  25.894  1.00 36.07
ATOM   133  O   ASP  1476      -12 830   5.842  27.066  1.00 36.26
ATOM   134  N   ARG  1477      -12.382   5.495  24.888  1.00 36.94
ATOM   136  CA  ARG  1477      -11.766   4.189  25.104  1.00 35.22
ATOM   137  CB  ARG  1477      -12.081   3.268  23.925  1.00 34.29
ATOM   138  CG  ARG  1477      -13.546   3.056  23.675  1.00 32.23
ATOM   139  CD  ARG  1477      -14.206   2.434  24.879  1.00 30.56
ATOM   140  NE  ARG  1477      -14.426   3.419  25.925  1.00 31.86
ATOM   142  CZ  ARG  1477      -14.730   3.126  27.182  1.00 33.09
ATOM   143  NH1 ARG  1477      -14.855   1.858  27.563  1.00 35.00
ATOM   146  NH2 ARG  1477      -14.904   4.101  28.053  1.00 29.62
ATOM   149  C   ARG  1477      -10.262   4.270  25.271  1.00 35.51
ATOM   150  O   ARG  1477       -9.621   3.290  25.637  1.00 36.44
ATOM   151  N   LEU  1478       -9.704   5.444  25.023  1.00 34.59
ATOM   153  CA  LEU  1478       -8.270   5.630  25.129  1.00 36.35
ATOM   154  CB  LEU  1478       -7.750   6.254  23.840  1.00 36.41
ATOM   155  CG  LEU  1478       -6.250   6.185  23.556  1.00 37.19
ATOM   156  CD1 LEU  1478       -5.791   4.728  23.479  1.00 34.63
ATOM   157  CD2 LEU  1478       -5.959   6.914  22.251  1 00 34.88
ATOM   158  C   LEU  1478       -7.901   6.517  26.325  1.00 38.74
ATOM   159  O   LEU  1478       -8.146   7.733  26.309  1.00 41.20
ATOM   160  N   VAL  1479       -7.311   5.907  27.355  1.00 36.92
ATOM   162  CA  VAL  1479       -6.885   6.622  28.560  1.00 35.79
ATOM   163  CB  VAL  1479       -6.929   5.693  29.780  1.00 35.81
ATOM   164  CG1 VAL  1479       -6.579   6.453  31.032  1.00 40.11
ATOM   165  CG2 VAL  1479       -8.302   5.056  29.907  1.00 35.59
ATOM   166  C   VAL  1479       -5.438   7.118  28.362  1.00 36.60
ATOM   167  O   VAL  1479       -4.479   6.369  28.583  1.00 33.48
ATOM   168  N   LEU  1480       -5.282   8.372  27.938  1.00 39.09
ATOM   170  CA  LEU  1480       -3.949   8.932  27.675  1.00 42.05
ATOM   171  CB  LEU  1480       -4.040  10.277  26.952  1.00 41.08
ATOM   172  CG  LEU  1480       -4.633  10.286  25.529  1.00 39.28
ATOM   173  CD1 LEU  1480       -4.766  11.720  25.051  1.00 40.04
ATOM   174  CD2 LEU  1480       -3.758   9.489  24.582  1.00 39.66
ATOM   175  C   LEU  1480       -3.001   9.027  28.867  1.00 41.51
ATOM   176  O   LEU  1480       -3.312   9.637  29.886  1.00 41.73
ATOM   177  N   GLY  1481       -1.817   8.444  28.697  1.00 40.68
ATOM   179  CA  GLY  1481       -0.849   8.439  29.775  1.00 41.28
ATOM   180  C   GLY  1481        0.412   9.225  29.529  1.00 43.08
ATOM   181  O   GLY  1481        0.474  10.147  28.701  1.00 45.65
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 182 | N | LYS | 1482 | 1.481 | 8.825 | 30.219 | 1.00 | 42.54 |
| ATOM | 184 | CA | LYS | 1482 | 2.781 | 9.453 | 30.128 | 1.00 | 43.74 |
| ATOM | 185 | CB | LYS | 1482 | 3.670 | 8.842 | 31.229 | 1.00 | 46.34 |
| ATOM | 186 | CG | LYS | 1482 | 5.155 | 8.979 | 30.954 | 1.00 | 52.23 |
| ATOM | 187 | CD | LYS | 1482 | 5.867 | 7.716 | 31.382 | 1.00 | 56.63 |
| ATOM | 188 | CE | LYS | 1482 | 5.373 | 6.518 | 30.607 | 1.00 | 54.20 |
| ATOM | 189 | NZ | LYS | 1482 | 6.199 | 5.320 | 30.955 | 1.00 | 59.97 |
| ATOM | 193 | C | LYS | 1482 | 3.552 | 9.422 | 28.806 | 1.00 | 43.96 |
| ATOM | 194 | O | LYS | 1482 | 3.557 | 8.422 | 28.111 | 1.00 | 44.68 |
| ATOM | 195 | N | PRO | 1483 | 4.259 | 10.521 | 28.481 | 1.00 | 44.06 |
| ATOM | 196 | CD | PRO | 1483 | 4.339 | 11.798 | 29.208 | 1.00 | 43.53 |
| ATOM | 197 | CA | PRO | 1483 | 5.005 | 10.573 | 27.208 | 1.00 | 44.07 |
| ATOM | 198 | CB | PRO | 1483 | 5.590 | 12.004 | 27.281 | 1.00 | 43.17 |
| ATOM | 199 | CG | PRO | 1483 | 4.630 | 12.738 | 28.114 | 1.00 | 43.75 |
| ATOM | 200 | C | PRO | 1483 | 6.172 | 9.543 | 27.116 | 1.00 | 43.47 |
| ATOM | 201 | O | PRO | 1483 | 6.853 | 9.308 | 28.120 | 1.00 | 43.76 |
| ATOM | 202 | N | LEU | 1484 | 6.408 | 9.001 | 25.932 | 1.00 | 41.71 |
| ATOM | 204 | CA | LEU | 1484 | 7.512 | 8.045 | 25.663 | 1.00 | 38.05 |
| ATOM | 205 | CB | LEU | 1484 | 6.964 | 6.803 | 24.927 | 1.00 | 33.38 |
| ATOM | 206 | CG | LEU | 1484 | 6.001 | 5.992 | 25.770 | 1.00 | 31.95 |
| ATOM | 207 | CD1 | LEU | 1484 | 5.258 | 4.914 | 24.975 | 1.00 | 27.41 |
| ATOM | 208 | CD2 | LEU | 1484 | 6.750 | 5.396 | 26.953 | 1.00 | 29.64 |
| ATOM | 209 | C | LEU | 1484 | 8.603 | 8.710 | 24.855 | 1.00 | 40.09 |
| ATOM | 210 | O | LEU | 1484 | 8.334 | 9.499 | 23.960 | 1.00 | 41.74 |
| ATOM | 211 | N | GLY | 1485 | 9.843 | 8.387 | 25.197 | 1.00 | 43.19 |
| ATOM | 213 | CA | GLY | 1485 | 10.976 | 8.923 | 24.512 | 1.00 | 50.32 |
| ATOM | 214 | C | GLY | 1485 | 11.261 | 10.408 | 24.697 | 1.00 | 54.65 |
| ATOM | 215 | O | GLY | 1485 | 11.036 | 10.973 | 25.770 | 1.00 | 54.73 |
| ATOM | 216 | N | GLU | 1486 | 11.747 | 11.072 | 23.647 | 1.00 | 59.07 |
| ATOM | 218 | CA | GLU | 1486 | 12.081 | 12.483 | 23.666 | 1.00 | 61.01 |
| ATOM | 219 | CB | GLU | 1486 | 13.489 | 12.646 | 24.275 | 1.00 | 62.51 |
| ATOM | 220 | C | GLU | 1486 | 12.014 | 13.183 | 22.295 | 1.00 | 62.48 |
| ATOM | 221 | O | GLU | 1486 | 12.901 | 13.970 | 21.949 | 1.00 | 64.10 |
| ATOM | 222 | N | GLY | 1487 | 10.975 | 12.892 | 21.519 | 1.00 | 62.29 |
| ATOM | 224 | CA | GLY | 1487 | 10.792 | 13.522 | 20.236 | 1.00 | 59.87 |
| ATOM | 225 | C | GLY | 1487 | 11.469 | 12.881 | 19.044 | 1.00 | 58.88 |
| ATOM | 226 | O | GLY | 1487 | 11.447 | 13.426 | 17.950 | 1.00 | 60.19 |
| ATOM | 227 | N | ALA | 1488 | 12.073 | 11.714 | 19.239 | 1.00 | 57.19 |
| ATOM | 229 | CA | ALA | 1488 | 12.721 | 11.016 | 18.140 | 1.00 | 55.59 |
| ATOM | 230 | CB | ALA | 1488 | 13.477 | 9.804 | 18.663 | 1.00 | 56.35 |
| ATOM | 231 | C | ALA | 1488 | 11.690 | 10.601 | 17.112 | 1.00 | 54.96 |
| ATOM | 232 | O | ALA | 1488 | 11.927 | 10.626 | 15.913 | 1.00 | 56.42 |
| ATOM | 233 | N | PHE | 1489 | 10.509 | 10.241 | 17.598 | 1.00 | 54.99 |
| ATOM | 235 | CA | PHE | 1489 | 9.401 | 9.807 | 16.721 | 1.00 | 54.07 |
| ATOM | 236 | CB | PHE | 1489 | 8.857 | 8.454 | 17.162 | 1.00 | 51.18 |
| ATOM | 237 | CG | PHE | 1489 | 9.880 | 7.373 | 17.137 | 1.00 | 46.81 |
| ATOM | 238 | CD1 | PHE | 1489 | 10.641 | 7.093 | 18.271 | 1.00 | 46.81 |
| ATOM | 239 | CD2 | PHE | 1489 | 10.096 | 6.612 | 15.984 | 1.00 | 48.30 |
| ATOM | 240 | CE1 | PHE | 1489 | 11.585 | 6.090 | 18.262 | 1.00 | 47.41 |
| ATOM | 241 | CE2 | PHE | 1489 | 11.040 | 5.601 | 15.963 | 1.00 | 48.23 |
| ATOM | 242 | CZ | PHE | 1489 | 11.794 | 5.336 | 17.111 | 1.00 | 47.94 |
| ATOM | 243 | C | PHE | 1489 | 8.261 | 10.814 | 16.748 | 1.00 | 54.90 |

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ATOM    244  O    PHE  1489      7.199  10.565  16.184  1.00 59.10
ATOM    245  N    GLY  1490      8.431  11.908  17.504  1.00 53.55
ATOM    247  CA   GLY  1490      7.432  12.958  17.611  1.00 50.20
ATOM    248  C    GLY  1490      6.745  12.844  18.942  1.00 49.82
ATOM    249  O    GLY  1490      7.266  12.161  19.837  1.00 50.95
ATOM    250  N    GLN  1491      5.614  13.514  19.124  1.00 49.53
ATOM    252  CA   GLN  1491      4.922  13.441  20.395  1.00 49.16
ATOM    253  CB   GLN  1491      3.927  14.590  20.564  1.00 51.74
ATOM    254  CG   GLN  1491      3.439  14.796  21.994  1.00 64.00
ATOM    255  CD   GLN  1491      2.545  16.039  22.180  1.00 71.35
ATOM    256  OE1  GLN  1491      2.534  16.922  21.352  1.00 77.94
ATOM    257  NE2  GLN  1491      1.824  16.083  23.289  1.00 76.51
ATOM    260  C    GLN  1491      4.207  12.083  20.505  1.00 45.94
ATOM    261  O    GLN  1491      3.151  11.869  19.919  1.00 48.02
ATOM    262  N    VAL  1492      4.848  11.129  21.184  1.00 41.00
ATOM    264  CA   VAL  1492      4.293   9.810  21.421  1.00 37.44
ATOM    265  CB   VAL  1492      5.235   8.665  21.025  1.00 34.74
ATOM    266  CG1  VAL  1492      4.593   7.325  21.285  1.00 28.97
ATOM    267  CG2  VAL  1492      5.632   8.769  19.553  1.00 35.78
ATOM    268  C    VAL  1492      4.014   9.621  22.901  1.00 38.67
ATOM    269  O    VAL  1492      4.907   9.769  23.735  1.00 38.62
ATOM    270  N    VAL  1493      2.776   9.276  23.250  1.00 39.98
ATOM    272  CA   VAL  1493      2.423   9.062  24.653  1.00 37.79
ATOM    273  CB   VAL  1493      1.257   9.970  25.093  1.00 37.36
ATOM    274  CG1  VAL  1493      1.489  11.403  24.689  1.00 39.11
ATOM    275  CG2  VAL  1493     -0.074   9.480  24.555  1.00 38.99
ATOM    276  C    VAL  1493      2.052   7.603  24.877  1.00 36.38
ATOM    277  O    VAL  1493      1.759   6.874  23.945  1.00 37.73
ATOM    278  N    LEU  1494      2.094   7.176  26.123  1.00 35.42
ATOM    280  CA   LEU  1494      1.718   5.817  26.483  1.00 33.65
ATOM    281  CB   LEU  1494      2.536   5.291  27.670  1.00 29.88
ATOM    282  CG   LEU  1494      2.117   3.945  28.279  1.00 30.31
ATOM    283  CD1  LEU  1494      2.103   2.844  27.244  1.00 30.83
ATOM    284  CD2  LEU  1494      3.049   3.574  29.400  1.00 32.12
ATOM    285  C    LEU  1494      0.260   5.934  26.870  1.00 34.27
ATOM    286  O    LEU  1494     -0.168   6.994  27.348  1.00 34.85
ATOM    287  N    ALA  1495     -0.527   4.898  26.608  1.00 32.20
ATOM    289  CA   ALA  1495     -1.930   4.954  26.980  1.00 29.71
ATOM    290  CB   ALA  1495     -2.724   5.722  25.930  1.00 25.48
ATOM    291  C    ALA  1495     -2.499   3.567  27.183  1.00 28.85
ATOM    292  O    ALA  1495     -1.826   2.563  26.998  1.00 27.28
ATOM    293  N    GLU  1496     -3.743   3.519  27.615  1.00 32.20
ATOM    295  CA   GLU  1496     -4.413   2.250  27.824  1.00 33.34
ATOM    296  CB   GLU  1496     -4.735   2.063  29.301  1.00 35.65
ATOM    297  CG   GLU  1496     -3.521   1.962  30.198  1.00 39.14
ATOM    298  CD   GLU  1496     -3.899   2.045  31.663  1.00 42.57
ATOM    299  OE1  GLU  1496     -4.469   3.083  32.061  1.00 42.59
ATOM    300  OE2  GLU  1496     -3.646   1.069  32.407  1.00 42.76
ATOM    301  C    GLU  1496     -5.692   2.274  26.994  1.00 33.40
ATOM    302  O    GLU  1496     -6.439   3.261  27.017  1.00 34.36
ATOM    303  N    ALA  1497     -5.875   1.247  26.177  1.00 31.67
ATOM    305  CA   ALA  1497     -7.051   1.168  25.351  1.00 31.23
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 306 | CB | ALA | 1497 | -6.671 | 0.750 | 23.953 | 1.00 | 28.13 |
| ATOM | 307 | C | ALA | 1497 | -8.000 | 0.168 | 25.974 | 1.00 | 32.02 |
| ATOM | 308 | O | ALA | 1497 | -7.599 | -0.954 | 26.261 | 1.00 | 33.45 |
| ATOM | 309 | N | ILE | 1498 | -9.218 | 0.602 | 26.282 | 1.00 | 34.15 |
| ATOM | 311 | CA | ILE | 1498 | -10.222 | -0.294 | 26.854 | 1.00 | 35.89 |
| ATOM | 312 | CB | ILE | 1498 | -11.294 | 0.453 | 27.679 | 1.00 | 35.30 |
| ATOM | 313 | CG2 | ILE | 1498 | -12.267 | -0.551 | 28.300 | 1.00 | 32.95 |
| ATOM | 314 | CG1 | ILE | 1498 | -10.663 | 1.316 | 28.770 | 1.00 | 35.29 |
| ATOM | 315 | CD1 | ILE | 1498 | -11.656 | 2.262 | 29.419 | 1.00 | 31.69 |
| ATOM | 316 | C | ILE | 1498 | -10.953 | -0.929 | 25.680 | 1.00 | 38.79 |
| ATOM | 317 | O | ILE | 1498 | -11.571 | -0.227 | 24.877 | 1.00 | 37.46 |
| ATOM | 318 | N | GLY | 1499 | -10.859 | -2.245 | 25.559 | 1.00 | 43.14 |
| ATOM | 320 | CA | GLY | 1499 | -11.544 | -2.918 | 24.477 | 1.00 | 46.90 |
| ATOM | 321 | C | GLY | 1499 | -10.673 | -3.299 | 23.298 | 1.00 | 49.69 |
| ATOM | 322 | O | GLY | 1499 | -9.921 | -4.269 | 23.387 | 1.00 | 51.47 |
| ATOM | 323 | N | LEU | 1500 | -10.739 | -2.508 | 22.223 | 1.00 | 49.92 |
| ATOM | 325 | CA | LEU | 1500 | -10.003 | -2.765 | 20.973 | 1.00 | 49.62 |
| ATOM | 326 | CB | LEU | 1500 | -8.478 | -2.898 | 21.185 | 1.00 | 49.96 |
| ATOM | 327 | CG | LEU | 1500 | -7.504 | -1.703 | 21.167 | 1.00 | 49.26 |
| ATOM | 328 | CD1 | LEU | 1500 | -6.069 | -2.217 | 21.284 | 1.00 | 47.17 |
| ATOM | 329 | CD2 | LEU | 1500 | -7.638 | -0.883 | 19.899 | 1.00 | 47.80 |
| ATOM | 330 | C | LEU | 1500 | -10.535 | -4.027 | 20.275 | 1.00 | 49.49 |
| ATOM | 331 | O | LEU | 1500 | -10.480 | -5.145 | 20.806 | 1.00 | 47.99 |
| ATOM | 332 | N | PRO | 1505 | -13.253 | -5.837 | 25.284 | 1.00 | 50.58 |
| ATOM | 333 | CD | PRO | 1505 | -13.877 | -7.173 | 25.239 | 1.00 | 51.43 |
| ATOM | 334 | CA | PRO | 1505 | -14.197 | -4.825 | 25.779 | 1.00 | 48.08 |
| ATOM | 335 | CB | PRO | 1505 | -15.548 | -5.521 | 25.627 | 1.00 | 48.59 |
| ATOM | 336 | CG | PRO | 1505 | -15.216 | -6.944 | 25.940 | 1.00 | 51.66 |
| ATOM | 337 | C | PRO | 1505 | -13.904 | -4.396 | 27.227 | 1.00 | 44.58 |
| ATOM | 338 | O | PRO | 1505 | -13.883 | -3.202 | 27.531 | 1.00 | 42.73 |
| ATOM | 339 | N | ASN | 1506 | -13.640 | -5.363 | 28.102 | 1.00 | 42.10 |
| ATOM | 341 | CA | ASN | 1506 | -13.337 | -5.053 | 29.497 | 1.00 | 45.05 |
| ATOM | 342 | CB | ASN | 1506 | -14.202 | -5.893 | 30.434 | 1.00 | 47.04 |
| ATOM | 343 | CG | ASN | 1506 | -15.657 | -5.493 | 30.395 | 1.00 | 48.72 |
| ATOM | 344 | OD1 | ASN | 1506 | -15.999 | -4.309 | 30.487 | 1.00 | 50.48 |
| ATOM | 345 | ND2 | ASN | 1506 | -16.529 | -6.478 | 30.260 | 1.00 | 51.15 |
| ATOM | 348 | C | ASN | 1506 | -11.863 | -5.251 | 29.836 | 1.00 | 46.50 |
| ATOM | 349 | O | ASN | 1506 | -11.487 | -5.343 | 31.008 | 1.00 | 46.50 |
| ATOM | 350 | N | ARG | 1507 | -11.029 | -5.284 | 28.806 | 1.00 | 46.99 |
| ATOM | 352 | CA | ARG | 1507 | -9.594 | -5.466 | 28.976 | 1.00 | 47.52 |
| ATOM | 353 | CB | ARG | 1507 | -9.111 | -6.650 | 28.142 | 1.00 | 54.20 |
| ATOM | 354 | CG | ARG | 1507 | -9.327 | -7.993 | 28.781 | 1.00 | 64.52 |
| ATOM | 355 | CD | ARG | 1507 | -8.402 | -8.180 | 29.963 | 1.00 | 71.17 |
| ATOM | 356 | NE | ARG | 1507 | -8.592 | -9.494 | 30.556 | 1.00 | 76.52 |
| ATOM | 358 | CZ | ARG | 1507 | -8.030 | -9.898 | 31.689 | 1.00 | 81.64 |
| ATOM | 359 | NH1 | ARG | 1507 | -7.219 | -9.096 | 32.375 | 1.00 | 83.30 |
| ATOM | 362 | NH2 | ARG | 1507 | -8.340 | -11.093 | 32.174 | 1.00 | 84.44 |
| ATOM | 365 | C | ARG | 1507 | -8.871 | -4.234 | 28.485 | 1.00 | 43.46 |
| ATOM | 366 | O | ARG | 1507 | -9.227 | -3.695 | 27.440 | 1.00 | 42.73 |
| ATOM | 367 | N | VAL | 1508 | -7.912 | -3.749 | 29.265 | 1.00 | 40.84 |
| ATOM | 369 | CA | VAL | 1508 | -7.143 | -2.598 | 28.830 | 1.00 | 38.27 |
| ATOM | 370 | CB | VAL | 1508 | -6.786 | -1.604 | 29.961 | 1.00 | 34.90 |

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ATOM     371   CG1  VAL   1508        -8.038   -1.124   30.646   1.00  41.81
ATOM     372   CG2  VAL   1508        -5.850   -2.226   30.944   1.00  35.89
ATOM     373   C    VAL   1508        -5.874   -3.147   28.211   1.00  36.81
ATOM     374   O    VAL   1508        -5.371   -4.191   28.637   1.00  35.13
ATOM     375   N    THR   1509        -5.393   -2.465   27.180   1.00  36.04
ATOM     377   CA   THR   1509        -4.184   -2.854   26.485   1.00  33.31
ATOM     378   CB   THR   1509        -4.503   -3.254   25.025   1.00  33.79
ATOM     379   OG1  THR   1509        -5.511   -4.275   25.014   1.00  33.98
ATOM     381   CG2  THR   1509        -3.259   -3.774   24.321   1.00  32.78
ATOM     382   C    THR   1509        -3.268   -1.627   26.453   1.00  32.37
ATOM     383   O    THR   1509        -3.718   -0.533   26.113   1.00  31.97
ATOM     384   N    LYS   1510        -2.015   -1.786   26.884   1.00  32.96
ATOM     386   CA   LYS   1510        -1.071   -0.673   26.828   1.00  33.25
ATOM     387   CB   LYS   1510         0.157   -0.902   27.699   1.00  34.65
ATOM     388   CG   LYS   1510        -0.093   -0.909   29.197   1.00  39.64
ATOM     389   CD   LYS   1510         1.237   -1.105   29.913   1.00  43.51
ATOM     390   CE   LYS   1510         1.110   -1.949   31.173   1.00  48.42
ATOM     391   NZ   LYS   1510         0.399   -1.256   32.287   1.00  53.03
ATOM     395   C    LYS   1510        -0.646   -0.550   25.370   1.00  32.26
ATOM     396   O    LYS   1510        -0.240   -1.533   24.736   1.00  30.20
ATOM     397   N    VAL   1511        -0.760    0.665   24.849   1.00  32.28
ATOM     399   CA   VAL   1511        -0.436    0.980   23.472   1.00  30.73
ATOM     400   CB   VAL   1511        -1.738    1.140   22.666   1.00  32.25
ATOM     401   CG1  VAL   1511        -2.566   -0.147   22.723   1.00  29.00
ATOM     402   CG2  VAL   1511        -2.549    2.347   23.193   1.00  29.17
ATOM     403   C    VAL   1511         0.329    2.307   23.423   1.00  30.91
ATOM     404   O    VAL   1511         0.445    3.008   24.433   1.00  31.94
ATOM     405   N    ALA   1512         0.842    2.658   22.250   1.00  27.30
ATOM     407   CA   ALA   1512         1.550    3.914   22.094   1.00  24.22
ATOM     408   CB   ALA   1512         2.921    3.694   21.493   1.00  23.39
ATOM     409   C    ALA   1512         0.698    4.769   21.181   1.00  23.62
ATOM     410   O    ALA   1512         0.116    4.271   20.228   1.00  22.69
ATOM     411   N    VAL   1513         0.605    6.054   21.484   1.00  27.51
ATOM     413   CA   VAL   1513        -0.192    6.984   20.688   1.00  30.03
ATOM     414   CB   VAL   1513        -1.359    7.613   21.522   1.00  28.31
ATOM     415   CG1  VAL   1513        -2.218    8.522   20.650   1.00  28.93
ATOM     416   CG2  VAL   1513        -2.214    6.542   22.159   1.00  26.00
ATOM     417   C    VAL   1513         0.674    8.108   20.107   1.00  31.21
ATOM     418   O    VAL   1513         1.370    8.816   20.834   1.00  29.73
ATOM     419   N    LYS   1514         0.631    8.225   18.784   1.00  33.99
ATOM     421   CA   LYS   1514         1.342    9.258   18.037   1.00  35.44
ATOM     422   CB   LYS   1514         1.831    8.692   16.707   1.00  34.55
ATOM     423   CG   LYS   1514         2.835    7.586   16.872   1.00  35.38
ATOM     424   CD   LYS   1514         3.025    6.807   15.599   1.00  36.87
ATOM     425   CE   LYS   1514         3.457    7.710   14.438   1.00  45.19
ATOM     426   NZ   LYS   1514         4.598    8.622   14.755   1.00  44.31
ATOM     430   C    LYS   1514         0.304   10.345   17.761   1.00  35.97
ATOM     431   O    LYS   1514        -0.806   10.037   17.299   1.00  34.39
ATOM     432   N    MET   1515         0.673   11.596   18.028   1.00  38.17
ATOM     434   CA   MET   1515        -0.207   12.747   17.835   1.00  41.17
ATOM     435   CB   MET   1515        -0.901   13.098   19.145   1.00  39.54
ATOM     436   CG   MET   1515         0.075   13.428   20.255   1.00  39.11
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 437 | SD | MET | 1515 | -0.766 | 13.612 | 21.799 | 1.00 | 43.85 |
| ATOM | 438 | CE | MET | 1515 | -1.212 | 11.937 | 22.087 | 1.00 | 46.18 |
| ATOM | 439 | C | MET | 1515 | 0.612 | 13.939 | 17.391 | 1.00 | 43.65 |
| ATOM | 440 | O | MET | 1515 | 1.834 | 13.905 | 17.445 | 1.00 | 45.72 |
| ATOM | 441 | N | LEU | 1516 | -0.053 | 14.962 | 16.872 | 1.00 | 48.73 |
| ATOM | 443 | CA | LEU | 1516 | 0.640 | 16.175 | 16.448 | 1.00 | 52.23 |
| ATOM | 444 | CB | LEU | 1516 | -0.152 | 16.917 | 15.374 | 1.00 | 49.77 |
| ATOM | 445 | CG | LEU | 1516 | -0.413 | 16.254 | 14.036 | 1.00 | 48.04 |
| ATOM | 446 | CD1 | LEU | 1516 | -1.418 | 17.104 | 13.285 | 1.00 | 48.16 |
| ATOM | 447 | CD2 | LEU | 1516 | 0.884 | 16.102 | 13.265 | 1.00 | 42.80 |
| ATOM | 448 | C | LEU | 1516 | 0.810 | 17.119 | 17.631 | 1.00 | 55.67 |
| ATOM | 449 | O | LEU | 1516 | 0.217 | 16.927 | 18.703 | 1.00 | 53.99 |
| ATOM | 450 | N | LYS | 1517 | 1.580 | 18.174 | 17.402 | 1.00 | 60.97 |
| ATOM | 452 | CA | LYS | 1517 | 1.823 | 19.193 | 18.416 | 1.00 | 65.19 |
| ATOM | 453 | CB | LYS | 1517 | 3.274 | 19.668 | 18.344 | 1.00 | 69.34 |
| ATOM | 454 | CG | LYS | 1517 | 4.294 | 18.559 | 18.529 | 1.00 | 72.86 |
| ATOM | 455 | CD | LYS | 1517 | 5.646 | 18.935 | 17.929 | 1.00 | 74.91 |
| ATOM | 456 | CE | LYS | 1517 | 6.686 | 17.851 | 18.197 | 1.00 | 74.38 |
| ATOM | 457 | NZ | LYS | 1517 | 8.010 | 18.241 | 17.649 | 1.00 | 75.45 |
| ATOM | 461 | C | LYS | 1517 | 0.879 | 20.357 | 18.139 | 1.00 | 65.97 |
| ATOM | 462 | O | LYS | 1517 | 0.303 | 20.451 | 17.053 | 1.00 | 64.59 |
| ATOM | 463 | N | SER | 1518 | 0.776 | 21.270 | 19.098 | 1.00 | 68.20 |
| ATOM | 465 | CA | SER | 1518 | -0.107 | 22.422 | 18.972 | 1.00 | 71.92 |
| ATOM | 466 | CB | SER | 1518 | -0.002 | 23.322 | 20.202 | 1.00 | 69.89 |
| ATOM | 467 | C | SER | 1518 | 0.144 | 23.247 | 17.718 | 1.00 | 74.68 |
| ATOM | 468 | O | SER | 1518 | -0.798 | 23.604 | 17.006 | 1.00 | 77.44 |
| ATOM | 469 | N | ASP | 1519 | 1.417 | 23.493 | 17.422 | 1.00 | 76.04 |
| ATOM | 471 | CA | ASP | 1519 | 1.799 | 24.299 | 16.264 | 1.00 | 76.48 |
| ATOM | 472 | CB | ASP | 1519 | 3.126 | 25.011 | 16.539 | 1.00 | 77.59 |
| ATOM | 473 | C | ASP | 1519 | 1.912 | 23.525 | 14.958 | 1.00 | 75.88 |
| ATOM | 474 | O | ASP | 1519 | 2.374 | 24.075 | 13.959 | 1.00 | 77.52 |
| ATOM | 475 | N | ALA | 1520 | 1.486 | 22.265 | 14.956 | 1.00 | 74.39 |
| ATOM | 477 | CA | ALA | 1520 | 1.574 | 21.439 | 13.758 | 1.00 | 72.83 |
| ATOM | 478 | CB | ALA | 1520 | 0.930 | 20.079 | 14.010 | 1.00 | 73.06 |
| ATOM | 479 | C | ALA | 1520 | 0.889 | 22.153 | 12.598 | 1.00 | 71.47 |
| ATOM | 480 | O | ALA | 1520 | -0.096 | 22.858 | 12.797 | 1.00 | 73.48 |
| ATOM | 481 | N | THR | 1521 | 1.440 | 22.015 | 11.401 | 1.00 | 69.15 |
| ATOM | 483 | CA | THR | 1521 | 0.858 | 22.653 | 10.234 | 1.00 | 70.05 |
| ATOM | 484 | CB | THR | 1521 | 1.950 | 23.110 | 9.272 | 1.00 | 70.21 |
| ATOM | 485 | OG1 | THR | 1521 | 2.505 | 21.969 | 8.607 | 1.00 | 72.71 |
| ATOM | 487 | CG2 | THR | 1521 | 3.053 | 23.815 | 10.043 | 1.00 | 71.01 |
| ATOM | 488 | C | THR | 1521 | -0.015 | 21.616 | 9.550 | 1.00 | 70.64 |
| ATOM | 489 | O | THR | 1521 | 0.015 | 20.443 | 9.932 | 1.00 | 72.38 |
| ATOM | 490 | N | GLU | 1522 | -0.782 | 22.026 | 8.542 | 1.00 | 69.70 |
| ATOM | 492 | CA | GLU | 1522 | -1.623 | 21.081 | 7.815 | 1.00 | 67.41 |
| ATOM | 493 | CB | GLU | 1522 | -2.478 | 21.800 | 6.761 | 1.00 | 70.01 |
| ATOM | 494 | C | GLU | 1522 | -0.718 | 20.024 | 7.168 | 1.00 | 64.50 |
| ATOM | 495 | O | GLU | 1522 | -1.125 | 18.878 | 7.006 | 1.00 | 63.76 |
| ATOM | 496 | N | LYS | 1523 | 0.512 | 20.419 | 6.827 | 1.00 | 60.75 |
| ATOM | 498 | CA | LYS | 1523 | 1.483 | 19.502 | 6.240 | 1.00 | 58.57 |
| ATOM | 499 | CB | LYS | 1523 | 2.782 | 20.230 | 5.883 | 1.00 | 60.63 |
| ATOM | 500 | CG | LYS | 1523 | 3.909 | 19.318 | 5.361 | 1.00 | 62.47 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 501 | CD | LYS | 1523 | 3.459 | 18.461 | 4.168 | 1.00 | 63.35 |
| ATOM | 502 | CE | LYS | 1523 | 4.633 | 17.700 | 3.559 | 1.00 | 66.57 |
| ATOM | 503 | NZ | LYS | 1523 | 4.210 | 16.733 | 2.498 | 1.00 | 69.56 |
| ATOM | 507 | C | LYS | 1523 | 1.763 | 18.441 | 7.281 | 1.00 | 55.98 |
| ATOM | 508 | O | LYS | 1523 | 1.790 | 17.251 | 6.972 | 1.00 | 56.37 |
| ATOM | 509 | N | ASP | 1524 | 1.960 | 18.885 | 8.517 | 1.00 | 52.16 |
| ATOM | 511 | CA | ASP | 1524 | 2.211 | 17.980 | 9.630 | 1.00 | 48.91 |
| ATOM | 512 | CB | ASP | 1524 | 2.487 | 18.762 | 10.915 | 1.00 | 50.87 |
| ATOM | 513 | CG | ASP | 1524 | 3.865 | 19.401 | 10.928 | 1.00 | 53.00 |
| ATOM | 514 | OD1 | ASP | 1524 | 4.004 | 20.511 | 11.489 | 1.00 | 53.77 |
| ATOM | 515 | OD2 | ASP | 1524 | 4.816 | 18.785 | 10.394 | 1.00 | 56.30 |
| ATOM | 516 | C | ASP | 1524 | 1.032 | 17.031 | 9.831 | 1.00 | 45.34 |
| ATOM | 517 | O | ASP | 1524 | 1.221 | 15.858 | 10.176 | 1.00 | 45.63 |
| ATOM | 518 | N | LEU | 1525 | -0.176 | 17.530 | 9.593 | 1.00 | 40.15 |
| ATOM | 520 | CA | LEU | 1525 | -1.368 | 16.715 | 9.711 | 1.00 | 39.38 |
| ATOM | 521 | CB | LEU | 1525 | -2.624 | 17.588 | 9.633 | 1.00 | 41.66 |
| ATOM | 522 | CG | LEU | 1525 | -4.020 | 16.937 | 9.585 | 1.00 | 42.75 |
| ATOM | 523 | CD1 | LEU | 1525 | -4.245 | 15.945 | 10.727 | 1.00 | 42.97 |
| ATOM | 524 | CD2 | LEU | 1525 | -5.058 | 18.026 | 9.644 | 1.00 | 42.24 |
| ATOM | 525 | C | LEU | 1525 | -1.340 | 15.699 | 8.575 | 1.00 | 39.77 |
| ATOM | 526 | O | LEU | 1525 | -1.509 | 14.506 | 8.813 | 1.00 | 39.11 |
| ATOM | 527 | N | SER | 1526 | -1.062 | 16.172 | 7.361 | 1.00 | 39.64 |
| ATOM | 529 | CA | SER | 1526 | -0.998 | 15.320 | 6.181 | 1.00 | 40.65 |
| ATOM | 530 | CB | SER | 1526 | -0.541 | 16.105 | 4.947 | 1.00 | 43.32 |
| ATOM | 531 | OG | SER | 1526 | -1.398 | 17.190 | 4.656 | 1.00 | 52.41 |
| ATOM | 533 | C | SER | 1526 | -0.015 | 14.201 | 6.383 | 1.00 | 39.12 |
| ATOM | 534 | O | SER | 1526 | -0.346 | 13.038 | 6.198 | 1.00 | 41.75 |
| ATOM | 535 | N | ASP | 1527 | 1.203 | 14.553 | 6.769 | 1.00 | 38.30 |
| ATOM | 537 | CA | ASP | 1527 | 2.244 | 13.552 | 6.969 | 1.00 | 39.28 |
| ATOM | 538 | CB | ASP | 1527 | 3.531 | 14.208 | 7.471 | 1.00 | 41.16 |
| ATOM | 539 | CG | ASP | 1527 | 4.218 | 15.069 | 6.404 | 1.00 | 45.20 |
| ATOM | 540 | OD1 | ASP | 1527 | 3.861 | 14.972 | 5.198 | 1.00 | 43.25 |
| ATOM | 541 | OD2 | ASP | 1527 | 5.132 | 15.840 | 6.788 | 1.00 | 45.93 |
| ATOM | 542 | C | ASP | 1527 | 1.788 | 12.443 | 7.903 | 1.00 | 37.34 |
| ATOM | 543 | O | ASP | 1527 | 1.867 | 11.259 | 7.557 | 1.00 | 37.24 |
| ATOM | 544 | N | LEU | 1528 | 1.224 | 12.935 | 9.036 | 1.00 | 35.88 |
| ATOM | 546 | CA | LEU | 1528 | 0.728 | 11.874 | 10.009 | 1.00 | 35.07 |
| ATOM | 547 | CB | LEU | 1528 | 0.185 | 12.606 | 11.242 | 1.00 | 34.38 |
| ATOM | 548 | CG | LEU | 1528 | -0.146 | 11.789 | 12.491 | 1.00 | 35.86 |
| ATOM | 549 | CD1 | LEU | 1528 | 1.009 | 10.845 | 12.820 | 1.00 | 34.83 |
| ATOM | 550 | CD2 | LEU | 1528 | -0.435 | 12.711 | 13.642 | 1.00 | 29.98 |
| ATOM | 551 | C | LEU | 1528 | -0.351 | 10.977 | 9.374 | 1.00 | 33.31 |
| ATOM | 552 | O | LEU | 1528 | -0.342 | 9.756 | 9.552 | 1.00 | 34.55 |
| ATOM | 553 | N | ILE | 1529 | -1.236 | 11.575 | 8.585 | 1.00 | 32.16 |
| ATOM | 555 | CA | ILE | 1529 | -2.306 | 10.829 | 7.924 | 1.00 | 30.94 |
| ATOM | 556 | CB | ILE | 1529 | -3.304 | 11.757 | 7.178 | 1.00 | 27.07 |
| ATOM | 557 | CG2 | ILE | 1529 | -4.388 | 10.926 | 6.521 | 1.00 | 26.06 |
| ATOM | 558 | CG1 | ILE | 1529 | -3.953 | 12.723 | 8.169 | 1.00 | 23.67 |
| ATOM | 559 | CD1 | ILE | 1529 | -4.877 | 13.736 | 7.526 | 1.00 | 22.34 |
| ATOM | 560 | C | ILE | 1529 | -1.684 | 9.856 | 6.947 | 1.00 | 31.34 |
| ATOM | 561 | O | ILE | 1529 | -2.058 | 8.683 | 6.912 | 1.00 | 33.57 |
| ATOM | 562 | N | SER | 1530 | -0.703 | 10.331 | 6.191 | 1.00 | 30.74 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 564 | CA | SER | 1530 | 0.007 | 9.496 | 5.230 | 1.00 | 32.04 |
| ATOM | 565 | CB | SER | 1530 | 1.109 | 10.302 | 4.548 | 1.00 | 35.20 |
| ATOM | 566 | OG | SER | 1530 | 0.596 | 11.501 | 4.002 | 1.00 | 41.97 |
| ATOM | 568 | C | SER | 1530 | 0.620 | 8.262 | 5.895 | 1.00 | 29.06 |
| ATOM | 569 | O | SER | 1530 | 0.478 | 7.140 | 5.377 | 1.00 | 26.64 |
| ATOM | 570 | N | GLU | 1531 | 1.287 | 8.464 | 7.034 | 1.00 | 23.86 |
| ATOM | 572 | CA | GLU | 1531 | 1.918 | 7.367 | 7.759 | 1.00 | 23.86 |
| ATOM | 573 | CB | GLU | 1531 | 2.729 | 7.893 | 8.944 | 1.00 | 25.69 |
| ATOM | 574 | CG | GLU | 1531 | 3.501 | 6.803 | 9.701 | 1.00 | 23.65 |
| ATOM | 575 | CD | GLU | 1531 | 4.341 | 7.319 | 10.868 | 1.00 | 26.03 |
| ATOM | 576 | OE1 | GLU | 1531 | 4.927 | 6.473 | 11.572 | 1.00 | 25.92 |
| ATOM | 577 | OE2 | GLU | 1531 | 4.435 | 8.549 | 11.094 | 1.00 | 26.55 |
| ATOM | 578 | C | GLU | 1531 | 0.906 | 6.325 | 8.222 | 1.00 | 25.44 |
| ATOM | 579 | O | GLU | 1531 | 1.200 | 5.126 | 8.228 | 1.00 | 23.67 |
| ATOM | 580 | N | MET | 1532 | -0.285 | 6.788 | 8.600 | 1.00 | 26.39 |
| ATOM | 582 | CA | MET | 1532 | -1.365 | 5.898 | 9.048 | 1.00 | 26.57 |
| ATOM | 583 | CB | MET | 1532 | -2.473 | 6.720 | 9.714 | 1.00 | 24.81 |
| ATOM | 584 | CG | MET | 1532 | -3.645 | 5.889 | 10.191 | 1.00 | 27.47 |
| ATOM | 585 | SD | MET | 1532 | -4.969 | 6.899 | 10.860 | 1.00 | 28.43 |
| ATOM | 586 | CE | MET | 1532 | -5.178 | 8.102 | 9.576 | 1.00 | 24.45 |
| ATOM | 587 | C | MET | 1532 | -1.923 | 5.076 | 7.861 | 1.00 | 28.30 |
| ATOM | 588 | O | MET | 1532 | -2.048 | 3.850 | 7.933 | 1.00 | 27.95 |
| ATOM | 589 | N | GLU | 1533 | -2.221 | 5.760 | 6.762 | 1.00 | 28.95 |
| ATOM | 591 | CA | GLU | 1533 | -2.732 | 5.111 | 5.565 | 1.00 | 30.32 |
| ATOM | 592 | CB | GLU | 1533 | -2.983 | 6.143 | 4.476 | 1.00 | 25.40 |
| ATOM | 593 | CG | GLU | 1533 | -4.064 | 7.127 | 4.852 | 1.00 | 26.09 |
| ATOM | 594 | CD | GLU | 1533 | -5.402 | 6.461 | 5.119 | 1.00 | 25.89 |
| ATOM | 595 | OE1 | GLU | 1533 | -5.913 | 5.745 | 4.240 | 1.00 | 27.24 |
| ATOM | 596 | OE2 | GLU | 1533 | -5.964 | 6.662 | 6.209 | 1.00 | 30.00 |
| ATOM | 597 | C | GLU | 1533 | -1.723 | 4.089 | 5.093 | 1.00 | 31.64 |
| ATOM | 598 | O | GLU | 1533 | -2.080 | 2.983 | 4.706 | 1.00 | 33.57 |
| ATOM | 599 | N | MET | 1534 | -0.455 | 4.472 | 5.166 | 1.00 | 33.57 |
| ATOM | 601 | CA | MET | 1534 | 0.664 | 3.618 | 4.793 | 1.00 | 32.86 |
| ATOM | 602 | CB | MET | 1534 | 1.957 | 4.390 | 5.003 | 1.00 | 32.89 |
| ATOM | 603 | CG | MET | 1534 | 3.159 | 3.559 | 4.851 | 1.00 | 39.27 |
| ATOM | 604 | SD | MET | 1534 | 3.577 | 3.513 | 3.164 | 1.00 | 51.24 |
| ATOM | 605 | CE | MET | 1534 | 5.153 | 4.319 | 3.204 | 1.00 | 44.97 |
| ATOM | 606 | C | MET | 1534 | 0.670 | 2.373 | 5.681 | 1.00 | 31.84 |
| ATOM | 607 | O | MET | 1534 | 0.816 | 1.250 | 5.198 | 1.00 | 33.78 |
| ATOM | 608 | N | MET | 1535 | 0.509 | 2.571 | 6.982 | 1.00 | 30.36 |
| ATOM | 610 | CA | MET | 1535 | 0.469 | 1.453 | 7.902 | 1.00 | 28.83 |
| ATOM | 611 | CB | MET | 1535 | 0.419 | 1.946 | 9.352 | 1.00 | 24.75 |
| ATOM | 612 | CG | MET | 1535 | 1.717 | 2.540 | 9.850 | 1.00 | 21.50 |
| ATOM | 613 | SD | MET | 1535 | 1.722 | 2.764 | 11.628 | 1.00 | 22.97 |
| ATOM | 614 | CE | MET | 1535 | 1.681 | 4.534 | 11.727 | 1.00 | 23.90 |
| ATOM | 615 | C | MET | 1535 | -0.725 | 0.540 | 7.572 | 1.00 | 30.33 |
| ATOM | 616 | O | MET | 1535 | -0.636 | -0.694 | 7.706 | 1.00 | 33.31 |
| ATOM | 617 | N | LYS | 1536 | -1.823 | 1.135 | 7.104 | 1.00 | 28.91 |
| ATOM | 619 | CA | LYS | 1536 | -3.011 | 0.364 | 6.732 | 1.00 | 28.07 |
| ATOM | 620 | CB | LYS | 1536 | -4.176 | 1.289 | 6.413 | 1.00 | 25.52 |
| ATOM | 621 | CG | LYS | 1536 | -4.689 | 2.080 | 7.579 | 1.00 | 21.46 |
| ATOM | 622 | CD | LYS | 1536 | -5.810 | 2.979 | 7.127 | 1.00 | 19.89 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 623 | CE | LYS | 1536 | -6.414 | 3.717 | 8.288 | 1.00 | 23.50 |
| ATOM | 624 | NZ | LYS | 1536 | -7.469 | 4.668 | 7.850 | 1.00 | 23.53 |
| ATOM | 628 | C | LYS | 1536 | -2.765 | -0.542 | 5.530 | 1.00 | 29.09 |
| ATOM | 629 | O | LYS | 1536 | -3.127 | -1.708 | 5.550 | 1.00 | 34.02 |
| ATOM | 630 | N | MET | 1537 | -2.141 | -0.009 | 4.488 | 1.00 | 29.03 |
| ATOM | 632 | CA | MET | 1537 | -1.869 | -0.792 | 3.288 | 1.00 | 30.13 |
| ATOM | 633 | CB | MET | 1537 | -1.315 | 0.111 | 2.177 | 1.00 | 31.96 |
| ATOM | 634 | CG | MET | 1537 | -2.304 | 1.114 | 1.589 | 1.00 | 35.15 |
| ATOM | 635 | SD | MET | 1537 | -3.757 | 0.380 | 0.787 | 1.00 | 41.18 |
| ATOM | 636 | CE | MET | 1537 | -3.026 | -0.360 | -0.666 | 1.00 | 43.05 |
| ATOM | 637 | C | MET | 1537 | -0.905 | -1.946 | 3.531 | 1.00 | 30.22 |
| ATOM | 638 | O | MET | 1537 | -1.118 | -3.051 | 3.045 | 1.00 | 30.88 |
| ATOM | 639 | N | ILE | 1538 | 0.164 | -1.686 | 4.275 | 1.00 | 30.91 |
| ATOM | 641 | CA | ILE | 1538 | 1.192 | -2.701 | 4.536 | 1.00 | 30.29 |
| ATOM | 642 | CB | ILE | 1538 | 2.429 | -2.082 | 5.221 | 1.00 | 28.64 |
| ATOM | 643 | CG2 | ILE | 1538 | 3.493 | -3.142 | 5.453 | 1.00 | 29.84 |
| ATOM | 644 | CG1 | ILE | 1538 | 3.025 | -1.030 | 4.287 | 1.00 | 32.82 |
| ATOM | 645 | CD1 | ILE | 1538 | 4.358 | -0.446 | 4.763 | 1.00 | 38.38 |
| ATOM | 646 | C | ILE | 1538 | 0.759 | -4.000 | 5.237 | 1.00 | 29.07 |
| ATOM | 647 | O | ILE | 1538 | 1.229 | -5.078 | 4.876 | 1.00 | 28.30 |
| ATOM | 648 | N | GLY | 1539 | -0.178 | -3.925 | 6.174 | 1.00 | 27.61 |
| ATOM | 650 | CA | GLY | 1539 | -0.592 | -5.147 | 6.849 | 1.00 | 26.22 |
| ATOM | 651 | C | GLY | 1539 | 0.273 | -5.484 | 8.055 | 1.00 | 25.67 |
| ATOM | 652 | O | GLY | 1539 | 1.345 | -4.906 | 8.241 | 1.00 | 28.05 |
| ATOM | 653 | N | LYS | 1540 | -0.150 | -6.483 | 8.819 | 1.00 | 23.80 |
| ATOM | 655 | CA | LYS | 1540 | 0.532 | -6.876 | 10.046 | 1.00 | 21.77 |
| ATOM | 656 | CB | LYS | 1540 | -0.491 | -7.436 | 11.045 | 1.00 | 20.04 |
| ATOM | 657 | CG | LYS | 1540 | -1.505 | -6.435 | 11.480 | 1.00 | 24.45 |
| ATOM | 658 | CD | LYS | 1540 | -2.472 | -6.997 | 12.488 | 1.00 | 32.57 |
| ATOM | 659 | CE | LYS | 1540 | -3.516 | -5.946 | 12.882 | 1.00 | 35.05 |
| ATOM | 660 | NZ | LYS | 1540 | -2.959 | -4.850 | 13.733 | 1.00 | 39.81 |
| ATOM | 664 | C | LYS | 1540 | 1.669 | -7.862 | 9.958 | 1.00 | 20.19 |
| ATOM | 665 | O | LYS | 1540 | 1.671 | -8.738 | 9.099 | 1.00 | 21.80 |
| ATOM | 666 | N | HIS | 1541 | 2.626 | -7.722 | 10.876 | 1.00 | 19.98 |
| ATOM | 668 | CA | HIS | 1541 | 3.770 | -8.626 | 11.000 | 1.00 | 22.43 |
| ATOM | 669 | CB | HIS | 1541 | 4.854 | -8.374 | 9.965 | 1.00 | 22.34 |
| ATOM | 670 | CG | HIS | 1541 | 5.892 | -9.455 | 9.923 | 1.00 | 20.68 |
| ATOM | 671 | CD2 | HIS | 1541 | 5.906 | -10.654 | 9.295 | 1.00 | 20.60 |
| ATOM | 672 | ND1 | HIS | 1541 | 7.074 | -9.382 | 10.633 | 1.00 | 23.67 |
| ATOM | 674 | CE1 | HIS | 1541 | 7.771 | -10.490 | 10.444 | 1.00 | 23.35 |
| ATOM | 675 | NE2 | HIS | 1541 | 7.087 | -11.278 | 9.634 | 1.00 | 22.04 |
| ATOM | 677 | C | HIS | 1541 | 4.385 | -8.477 | 12.376 | 1.00 | 27.21 |
| ATOM | 678 | O | HIS | 1541 | 4.538 | -7.367 | 12.885 | 1.00 | 31.33 |
| ATOM | 679 | N | LYS | 1542 | 4.726 | -9.619 | 12.958 | 1.00 | 29.25 |
| ATOM | 681 | CA | LYS | 1542 | 5.319 | -9.698 | 14.285 | 1.00 | 30.39 |
| ATOM | 682 | CB | LYS | 1542 | 5.660 | -11.151 | 14.610 | 1.00 | 33.76 |
| ATOM | 683 | CG | LYS | 1542 | 6.232 | -11.370 | 15.994 | 1.00 | 42.16 |
| ATOM | 684 | CD | LYS | 1542 | 6.400 | -12.833 | 16.230 | 1.00 | 49.69 |
| ATOM | 685 | CE | LYS | 1542 | 7.040 | -13.499 | 14.988 | 1.00 | 57.71 |
| ATOM | 686 | NZ | LYS | 1542 | 7.499 | -14.904 | 15.237 | 1.00 | 62.05 |
| ATOM | 690 | C | LYS | 1542 | 6.515 | -8.808 | 14.462 | 1.00 | 27.21 |
| ATOM | 691 | O | LYS | 1542 | 6.690 | -8.232 | 15.522 | 1.00 | 29.68 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 692 | N | ASN | 1543 | 7.293 | -8.619 | 13.410 | 1.00 | 23.81 |
| ATOM | 694 | CA | ASN | 1543 | 8.472 | -7.787 | 13.537 | 1.00 | 24.70 |
| ATOM | 695 | CB | ASN | 1543 | 9.697 | -8.550 | 13.031 | 1.00 | 24.68 |
| ATOM | 696 | CG | ASN | 1543 | 9.914 | -9.855 | 13.793 | 1.00 | 24.82 |
| ATOM | 697 | OD1 | ASN | 1543 | 9.734 | -10.942 | 13.239 | 1.00 | 27.33 |
| ATOM | 698 | ND2 | ASN | 1543 | 10.255 | -9.758 | 15.078 | 1.00 | 16.75 |
| ATOM | 701 | C | ASN | 1543 | 8.444 | -6.326 | 13.032 | 1.00 | 24.93 |
| ATOM | 702 | O | ASN | 1543 | 9.469 | -5.781 | 12.623 | 1.00 | 26.76 |
| ATOM | 703 | N | ILE | 1544 | 7.276 | -5.692 | 13.088 | 1.00 | 24.21 |
| ATOM | 705 | CA | ILE | 1544 | 7.121 | -4.281 | 12.710 | 1.00 | 21.87 |
| ATOM | 706 | CB | ILE | 1544 | 6.626 | -4.095 | 11.240 | 1.00 | 23.23 |
| ATOM | 707 | CG2 | ILE | 1544 | 7.549 | -4.837 | 10.267 | 1.00 | 23.87 |
| ATOM | 708 | CG1 | ILE | 1544 | 5.182 | -4.580 | 11.063 | 1.00 | 22.57 |
| ATOM | 709 | CD1 | ILE | 1544 | 4.639 | -4.342 | 9.659 | 1.00 | 17.59 |
| ATOM | 710 | C | ILE | 1544 | 6.122 | -3.656 | 13.696 | 1.00 | 21.64 |
| ATOM | 711 | O | ILE | 1544 | 5.399 | -4.377 | 14.397 | 1.00 | 21.00 |
| ATOM | 712 | N | ILE | 1545 | 6.167 | -2.340 | 13.856 | 1.00 | 21.59 |
| ATOM | 714 | CA | ILE | 1545 | 5.214 | -1.687 | 14.746 | 1.00 | 24.05 |
| ATOM | 715 | CB | ILE | 1545 | 5.641 | -0.242 | 15.138 | 1.00 | 23.68 |
| ATOM | 716 | CG2 | ILE | 1545 | 4.473 | 0.500 | 15.831 | 1.00 | 21.90 |
| ATOM | 717 | CG1 | ILE | 1545 | 6.880 | -0.284 | 16.050 | 1.00 | 21.94 |
| ATOM | 718 | CD1 | ILE | 1545 | 6.643 | -0.808 | 17.446 | 1.00 | 9.18 |
| ATOM | 719 | C | ILE | 1545 | 3.914 | -1.641 | 13.955 | 1.00 | 25.08 |
| ATOM | 720 | O | ILE | 1545 | 3.842 | -1.001 | 12.897 | 1.00 | 26.68 |
| ATOM | 721 | N | ASN | 1546 | 2.909 | -2.358 | 14.455 | 1.00 | 25.88 |
| ATOM | 723 | CA | ASN | 1546 | 1.602 | -2.424 | 13.800 | 1.00 | 24.61 |
| ATOM | 724 | CB | ASN | 1546 | 0.944 | -3.793 | 14.005 | 1.00 | 23.18 |
| ATOM | 725 | CG | ASN | 1546 | 1.759 | -4.923 | 13.434 | 1.00 | 21.54 |
| ATOM | 726 | OD1 | ASN | 1546 | 1.884 | -5.059 | 12.214 | 1.00 | 21.52 |
| ATOM | 727 | ND2 | ASN | 1546 | 2.319 | -5.748 | 14.313 | 1.00 | 18.83 |
| ATOM | 730 | C | ASN | 1546 | 0.646 | -1.368 | 14.292 | 1.00 | 23.02 |
| ATOM | 731 | O | ASN | 1546 | 0.739 | -0.911 | 15.429 | 1.00 | 25.66 |
| ATOM | 732 | N | LEU | 1547 | -0.285 | -1.014 | 13.422 | 1.00 | 24.45 |
| ATOM | 734 | CA | LEU | 1547 | -1.336 | -0.041 | 13.692 | 1.00 | 24.27 |
| ATOM | 735 | CB | LEU | 1547 | -1.819 | 0.553 | 12.360 | 1.00 | 18.04 |
| ATOM | 736 | CG | LEU | 1547 | -3.012 | 1.515 | 12.343 | 1.00 | 19.96 |
| ATOM | 737 | CD1 | LEU | 1547 | -2.630 | 2.928 | 12.842 | 1.00 | 10.60 |
| ATOM | 738 | CD2 | LEU | 1547 | -3.555 | 1.570 | 10.924 | 1.00 | 16.44 |
| ATOM | 739 | C | LEU | 1547 | -2.469 | -0.826 | 14.384 | 1.00 | 26.95 |
| ATOM | 740 | O | LEU | 1547 | -2.835 | -1.934 | 13.956 | 1.00 | 27.38 |
| ATOM | 741 | N | LEU | 1548 | -2.998 | -0.260 | 15.460 | 1.00 | 26.61 |
| ATOM | 743 | CA | LEU | 1548 | -4.063 | -0.902 | 16.222 | 1.00 | 26.25 |
| ATOM | 744 | CB | LEU | 1548 | -3.717 | -0.951 | 17.721 | 1.00 | 22.48 |
| ATOM | 745 | CG | LEU | 1548 | -2.370 | -1.553 | 18.117 | 1.00 | 20.24 |
| ATOM | 746 | CD1 | LEU | 1548 | -2.282 | -1.656 | 19.616 | 1.00 | 19.27 |
| ATOM | 747 | CD2 | LEU | 1548 | -2.175 | -2.929 | 17.492 | 1.00 | 19.23 |
| ATOM | 748 | C | LEU | 1548 | -5.401 | -0.198 | 16.017 | 1.00 | 26.75 |
| ATOM | 749 | O | LEU | 1548 | -6.447 | -0.837 | 16.036 | 1.00 | 25.56 |
| ATOM | 750 | N | GLY | 1549 | -5.367 | 1.115 | 15.823 | 1.00 | 25.78 |
| ATOM | 752 | CA | GLY | 1549 | -6.607 | 1.843 | 15.616 | 1.00 | 25.80 |
| ATOM | 753 | C | GLY | 1549 | -6.319 | 3.324 | 15.490 | 1.00 | 27.76 |
| ATOM | 754 | O | GLY | 1549 | -5.148 | 3.716 | 15.405 | 1.00 | 28.05 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 755 | N | ALA | 1550 | -7.369 | 4.143 | 15.530 | 1.00 | 27.34 |
| ATOM | 757 | CA | ALA | 1550 | -7.212 | 5.582 | 15.414 | 1.00 | 25.85 |
| ATOM | 758 | CB | ALA | 1550 | -6.925 | 5.947 | 13.978 | 1.00 | 23.09 |
| ATOM | 759 | C | ALA | 1550 | -8.430 | 6.353 | 15.897 | 1.00 | 26.58 |
| ATOM | 760 | O | ALA | 1550 | -9.562 | 5.866 | 15.797 | 1.00 | 28.26 |
| ATOM | 761 | N | CYS | 1551 | -8.182 | 7.551 | 16.429 | 1.00 | 26.30 |
| ATOM | 763 | CA | CYS | 1551 | -9.227 | 8.471 | 16.899 | 1.00 | 28.29 |
| ATOM | 764 | CB | CYS | 1551 | -8.966 | 8.952 | 18.342 | 1.00 | 27.12 |
| ATOM | 765 | SG | CYS | 1551 | -9.101 | 7.681 | 19.630 | 1.00 | 27.09 |
| ATOM | 766 | C | CYS | 1551 | -9.092 | 9.646 | 15.934 | 1.00 | 28.57 |
| ATOM | 767 | O | CYS | 1551 | -8.156 | 10.436 | 16.044 | 1.00 | 26.80 |
| ATOM | 768 | N | THR | 1552 | -9.966 | 9.699 | 14.933 | 1.00 | 29.27 |
| ATOM | 770 | CA | THR | 1552 | -9.889 | 10.736 | 13.921 | 1.00 | 29.30 |
| ATOM | 771 | CB | THR | 1552 | -9.779 | 10.110 | 12.495 | 1.00 | 27.19 |
| ATOM | 772 | OG1 | THR | 1552 | -10.978 | 9.393 | 12.191 | 1.00 | 26.68 |
| ATOM | 774 | CG2 | THR | 1552 | -8.629 | 9.133 | 12.414 | 1.00 | 27.00 |
| ATOM | 775 | C | THR | 1552 | -11.045 | 11.716 | 13.905 | 1.00 | 29.86 |
| ATOM | 776 | O | THR | 1552 | -10.918 | 12.838 | 13.403 | 1.00 | 30.69 |
| ATOM | 777 | N | GLN | 1553 | -12.201 | 11.268 | 14.369 | 1.00 | 31.21 |
| ATOM | 779 | CA | GLN | 1553 | -13.374 | 12.124 | 14.329 | 1.00 | 34.31 |
| ATOM | 780 | CB | GLN | 1553 | -14.641 | 11.279 | 14.147 | 1.00 | 33.00 |
| ATOM | 781 | CG | GLN | 1553 | -14.714 | 10.530 | 12.820 | 1.00 | 34.68 |
| ATOM | 782 | CD | GLN | 1553 | -14.584 | 11.453 | 11.617 | 1.00 | 39.26 |
| ATOM | 783 | OE1 | GLN | 1553 | -15.300 | 12.449 | 11.506 | 1.00 | 43.55 |
| ATOM | 784 | NE2 | GLN | 1553 | -13.668 | 11.129 | 10.718 | 1.00 | 37.56 |
| ATOM | 787 | C | GLN | 1553 | -13.502 | 13.040 | 15.526 | 1.00 | 36.86 |
| ATOM | 788 | O | GLN | 1553 | -13.030 | 12.714 | 16.613 | 1.00 | 34.88 |
| ATOM | 789 | N | ASP | 1554 | -14.122 | 14.195 | 15.290 | 1.00 | 40.73 |
| ATOM | 791 | CA | ASP | 1554 | -14.369 | 15.202 | 16.313 | 1.00 | 42.49 |
| ATOM | 792 | CB | ASP | 1554 | -15.693 | 14.913 | 17.028 | 1.00 | 46.26 |
| ATOM | 793 | CG | ASP | 1554 | -16.907 | 15.174 | 16.153 | 1.00 | 51.14 |
| ATOM | 794 | OD1 | ASP | 1554 | -17.686 | 16.097 | 16.488 | 1.00 | 57.62 |
| ATOM | 795 | OD2 | ASP | 1554 | -17.092 | 14.463 | 15.146 | 1.00 | 55.72 |
| ATOM | 796 | C | ASP | 1554 | -13.249 | 15.299 | 17.336 | 1.00 | 42.31 |
| ATOM | 797 | O | ASP | 1554 | -13.443 | 14.955 | 18.501 | 1.00 | 43.61 |
| ATOM | 798 | N | GLY | 1555 | -12.077 | 15.753 | 16.902 | 1.00 | 41.03 |
| ATOM | 800 | CA | GLY | 1555 | -10.960 | 15.864 | 17.823 | 1.00 | 37.98 |
| ATOM | 801 | C | GLY | 1555 | -9.605 | 15.674 | 17.167 | 1.00 | 38.30 |
| ATOM | 802 | O | GLY | 1555 | -9.533 | 15.478 | 15.953 | 1.00 | 37.28 |
| ATOM | 803 | N | PRO | 1556 | -8.511 | 15.693 | 17.961 | 1.00 | 37.62 |
| ATOM | 804 | CD | PRO | 1556 | -8.575 | 15.755 | 19.429 | 1.00 | 37.23 |
| ATOM | 805 | CA | PRO | 1556 | -7.123 | 15.533 | 17.500 | 1.00 | 33.79 |
| ATOM | 806 | CB | PRO | 1556 | -6.296 | 15.748 | 18.773 | 1.00 | 33.33 |
| ATOM | 807 | CG | PRO | 1556 | -7.254 | 16.353 | 19.770 | 1.00 | 36.99 |
| ATOM | 808 | C | PRO | 1556 | -6.891 | 14.134 | 16.990 | 1.00 | 33.57 |
| ATOM | 809 | O | PRO | 1556 | -7.378 | 13.175 | 17.568 | 1.00 | 32.10 |
| ATOM | 810 | N | LEU | 1557 | -6.168 | 14.031 | 15.884 | 1.00 | 33.23 |
| ATOM | 812 | CA | LEU | 1557 | -5.859 | 12.745 | 15.300 | 1.00 | 34.20 |
| ATOM | 813 | CB | LEU | 1557 | -5.173 | 12.950 | 13.944 | 1.00 | 32.88 |
| ATOM | 814 | CG | LEU | 1557 | -4.674 | 11.716 | 13.183 | 1.00 | 29.78 |
| ATOM | 815 | CD1 | LEU | 1557 | -5.810 | 10.730 | 12.943 | 1.00 | 29.22 |
| ATOM | 816 | CD2 | LEU | 1557 | -4.085 | 12.161 | 11.880 | 1.00 | 28.17 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 817 | C | LEU | 1557 | -4.950 | 11.927 | 16.225 | 1.00 | 36.29 |
| ATOM | 818 | O | LEU | 1557 | -3.847 | 12.365 | 16.580 | 1.00 | 37.50 |
| ATOM | 819 | N | TYR | 1558 | -5.427 | 10.765 | 16.658 | 1.00 | 35.35 |
| ATOM | 821 | CA | TYR | 1558 | -4.619 | 9.890 | 17.495 | 1.00 | 33.09 |
| ATOM | 822 | CB | TYR | 1558 | -5.323 | 9.516 | 18.805 | 1.00 | 34.16 |
| ATOM | 823 | CG | TYR | 1558 | -5.363 | 10.629 | 19.806 | 1.00 | 34.40 |
| ATOM | 824 | CD1 | TYR | 1558 | -6.364 | 10.688 | 20.771 | 1.00 | 33.23 |
| ATOM | 825 | CE1 | TYR | 1558 | -6.438 | 11.747 | 21.663 | 1.00 | 34.52 |
| ATOM | 826 | CD2 | TYR | 1558 | -4.426 | 11.655 | 19.757 | 1.00 | 37.30 |
| ATOM | 827 | CE2 | TYR | 1558 | -4.488 | 12.715 | 20.640 | 1.00 | 38.44 |
| ATOM | 828 | CZ | TYR | 1558 | -5.494 | 12.762 | 21.587 | 1.00 | 36.17 |
| ATOM | 829 | OH | TYR | 1558 | -5.561 | 13.848 | 22.431 | 1.00 | 34.28 |
| ATOM | 831 | C | TYR | 1558 | -4.379 | 8.627 | 16.700 | 1.00 | 31.12 |
| ATOM | 832 | O | TYR | 1558 | -5.329 | 7.980 | 16.255 | 1.00 | 29.83 |
| ATOM | 833 | N | VAL | 1559 | -3.109 | 8.321 | 16.468 | 1.00 | 29.60 |
| ATOM | 835 | CA | VAL | 1559 | -2.727 | 7.115 | 15.753 | 1.00 | 27.08 |
| ATOM | 836 | CB | VAL | 1559 | -1.647 | 7.420 | 14.704 | 1.00 | 24.96 |
| ATOM | 837 | CG1 | VAL | 1559 | -1.281 | 6.149 | 13.926 | 1.00 | 24.36 |
| ATOM | 838 | CG2 | VAL | 1559 | -2.147 | 8.525 | 13.765 | 1.00 | 19.21 |
| ATOM | 839 | C | VAL | 1559 | -2.238 | 6.102 | 16.794 | 1.00 | 25.65 |
| ATOM | 840 | O | VAL | 1559 | -1.169 | 6.257 | 17.389 | 1.00 | 24.97 |
| ATOM | 841 | N | ILE | 1560 | -3.067 | 5.095 | 17.046 | 1.00 | 25.91 |
| ATOM | 843 | CA | ILE | 1560 | -2.777 | 4.062 | 18.042 | 1.00 | 26.94 |
| ATOM | 844 | CB | ILE | 1560 | -4.081 | 3.530 | 18.637 | 1.00 | 24.89 |
| ATOM | 845 | CG2 | ILE | 1560 | -3.785 | 2.744 | 19.900 | 1.00 | 17.89 |
| ATOM | 846 | CG1 | ILE | 1560 | -5.028 | 4.707 | 18.907 | 1.00 | 22.84 |
| ATOM | 847 | CD1 | ILE | 1560 | -6.450 | 4.304 | 19.163 | 1.00 | 22.51 |
| ATOM | 848 | C | ILE | 1560 | -1.955 | 2.896 | 17.467 | 1.00 | 30.61 |
| ATOM | 849 | O | ILE | 1560 | -2.445 | 2.111 | 16.636 | 1.00 | 31.41 |
| ATOM | 850 | N | VAL | 1561 | -0.698 | 2.811 | 17.890 | 1.00 | 30.26 |
| ATOM | 852 | CA | VAL | 1561 | 0.222 | 1.779 | 17.429 | 1.00 | 29.39 |
| ATOM | 853 | CB | VAL | 1561 | 1.466 | 2.437 | 16.730 | 1.00 | 30.18 |
| ATOM | 854 | CG1 | VAL | 1561 | 1.030 | 3.188 | 15.475 | 1.00 | 20.60 |
| ATOM | 855 | CG2 | VAL | 1561 | 2.148 | 3.415 | 17.675 | 1.00 | 32.91 |
| ATOM | 856 | C | VAL | 1561 | 0.662 | 0.870 | 18.588 | 1.00 | 27.40 |
| ATOM | 857 | O | VAL | 1561 | 0.323 | 1.128 | 19.742 | 1.00 | 29.33 |
| ATOM | 858 | N | GLU | 1562 | 1.381 | -0.209 | 18.279 | 1.00 | 24.75 |
| ATOM | 860 | CA | GLU | 1562 | 1.852 | -1.142 | 19.308 | 1.00 | 22.64 |
| ATOM | 861 | CB | GLU | 1562 | 2.426 | -2.410 | 18.676 | 1.00 | 17.97 |
| ATOM | 862 | CG | GLU | 1562 | 1.365 | -3.282 | 18.029 | 1.00 | 24.33 |
| ATOM | 863 | CD | GLU | 1562 | 1.909 | -4.552 | 17.383 | 1.00 | 26.80 |
| ATOM | 864 | OE1 | GLU | 1562 | 1.247 | -5.592 | 17.507 | 1.00 | 33.32 |
| ATOM | 865 | OE2 | GLU | 1562 | 2.974 | -4.538 | 16.722 | 1.00 | 25.62 |
| ATOM | 866 | C | GLU | 1562 | 2.885 | -0.534 | 20.259 | 1.00 | 25.09 |
| ATOM | 867 | O | GLU | 1562 | 3.638 | 0.355 | 19.899 | 1.00 | 23.82 |
| ATOM | 868 | N | TYR | 1563 | 2.897 | -1.023 | 21.491 | 1.00 | 28.01 |
| ATOM | 870 | CA | TYR | 1563 | 3.805 | -0.539 | 22.512 | 1.00 | 26.93 |
| ATOM | 871 | CB | TYR | 1563 | 3.045 | -0.428 | 23.829 | 1.00 | 27.19 |
| ATOM | 872 | CG | TYR | 1563 | 3.868 | 0.008 | 25.009 | 1.00 | 27.72 |
| ATOM | 873 | CD1 | TYR | 1563 | 4.581 | 1.196 | 24.976 | 1.00 | 30.61 |
| ATOM | 874 | CE1 | TYR | 1563 | 5.303 | 1.620 | 26.069 | 1.00 | 33.05 |
| ATOM | 875 | CD2 | TYR | 1563 | 3.908 | -0.753 | 26.176 | 1.00 | 25.77 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 876 | CE2 | TYR | 1563 | 4.626 | -0.344 | 27.267 | 1.00 | 26.81 |
| ATOM | 877 | CZ | TYR | 1563 | 5.329 | 0.845 | 27.210 | 1.00 | 32.81 |
| ATOM | 878 | OH | TYR | 1563 | 6.091 | 1.271 | 28.276 | 1.00 | 40.16 |
| ATOM | 880 | C | TYR | 1563 | 4.989 | -1.487 | 22.675 | 1.00 | 28.73 |
| ATOM | 881 | O | TYR | 1563 | 4.815 | -2.704 | 22.735 | 1.00 | 27.05 |
| ATOM | 882 | N | ALA | 1564 | 6.189 | -0.908 | 22.743 | 1.00 | 29.89 |
| ATOM | 884 | CA | ALA | 1564 | 7.453 | -1.634 | 22.916 | 1.00 | 28.50 |
| ATOM | 885 | CB | ALA | 1564 | 8.392 | -1.349 | 21.721 | 1.00 | 27.54 |
| ATOM | 886 | C | ALA | 1564 | 8.036 | -1.092 | 24.229 | 1.00 | 27.05 |
| ATOM | 887 | O | ALA | 1564 | 8.790 | -0.129 | 24.249 | 1.00 | 31.20 |
| ATOM | 888 | N | SER | 1565 | 7.650 | -1.706 | 25.333 | 1.00 | 27.11 |
| ATOM | 890 | CA | SER | 1565 | 8.062 | -1.251 | 26.652 | 1.00 | 28.91 |
| ATOM | 891 | CB | SER | 1565 | 7.501 | -2.152 | 27.729 | 1.00 | 27.33 |
| ATOM | 892 | OG | SER | 1565 | 8.108 | -3.419 | 27.650 | 1.00 | 26.58 |
| ATOM | 894 | C | SER | 1565 | 9.530 | -1.085 | 26.915 | 1.00 | 30.19 |
| ATOM | 895 | O | SER | 1565 | 9.897 | -0.330 | 27.810 | 1.00 | 33.44 |
| ATOM | 896 | N | LYS | 1566 | 10.368 | -1.801 | 26.178 | 1.00 | 30.99 |
| ATOM | 898 | CA | LYS | 1566 | 11.798 | -1.708 | 26.410 | 1.00 | 30.50 |
| ATOM | 899 | CB | LYS | 1566 | 12.452 | -3.082 | 26.335 | 1.00 | 30.38 |
| ATOM | 900 | CG | LYS | 1566 | 12.037 | -3.943 | 27.507 | 1.00 | 27.83 |
| ATOM | 901 | CD | LYS | 1566 | 12.605 | -5.339 | 27.457 | 1.00 | 32.36 |
| ATOM | 902 | CE | LYS | 1566 | 12.345 | -6.024 | 28.784 | 1.00 | 30.57 |
| ATOM | 903 | NZ | LYS | 1566 | 12.651 | -7.460 | 28.722 | 1.00 | 34.82 |
| ATOM | 907 | C | LYS | 1566 | 12.526 | -0.678 | 25.573 | 1.00 | 30.39 |
| ATOM | 908 | O | LYS | 1566 | 13.755 | -0.567 | 25.640 | 1.00 | 32.53 |
| ATOM | 909 | N | GLY | 1567 | 11.753 | 0.127 | 24.851 | 1.00 | 29.45 |
| ATOM | 911 | CA | GLY | 1567 | 12.319 | 1.184 | 24.035 | 1.00 | 29.17 |
| ATOM | 912 | C | GLY | 1567 | 13.079 | 0.742 | 22.806 | 1.00 | 28.14 |
| ATOM | 913 | O | GLY | 1567 | 12.875 | -0.364 | 22.324 | 1.00 | 27.70 |
| ATOM | 914 | N | ASN | 1568 | 13.975 | 1.601 | 22.320 | 1.00 | 29.48 |
| ATOM | 916 | CA | ASN | 1568 | 14.754 | 1.308 | 21.121 | 1.00 | 30.00 |
| ATOM | 917 | CB | ASN | 1568 | 15.271 | 2.591 | 20.464 | 1.00 | 28.53 |
| ATOM | 918 | CG | ASN | 1568 | 16.342 | 3.285 | 21.281 | 1.00 | 30.13 |
| ATOM | 919 | OD1 | ASN | 1568 | 17.305 | 2.670 | 21.730 | 1.00 | 31.50 |
| ATOM | 920 | ND2 | ASN | 1568 | 16.212 | 4.591 | 21.420 | 1.00 | 30.91 |
| ATOM | 923 | C | ASN | 1568 | 15.892 | 0.333 | 21.352 | 1.00 | 28.83 |
| ATOM | 924 | O | ASN | 1568 | 16.371 | 0.201 | 22.472 | 1.00 | 29.87 |
| ATOM | 925 | N | LEU | 1569 | 16.346 | -0.300 | 20.274 | 1.00 | 27.43 |
| ATOM | 927 | CA | LEU | 1569 | 17.417 | -1.291 | 20.323 | 1.00 | 29.95 |
| ATOM | 928 | CB | LEU | 1569 | 17.511 | -2.022 | 18.972 | 1.00 | 28.96 |
| ATOM | 929 | CG | LEU | 1569 | 18.508 | -3.173 | 18.797 | 1.00 | 30.82 |
| ATOM | 930 | CD1 | LEU | 1569 | 18.431 | -4.211 | 19.939 | 1.00 | 28.31 |
| ATOM | 931 | CD2 | LEU | 1569 | 18.244 | -3.819 | 17.461 | 1.00 | 25.70 |
| ATOM | 932 | C | LEU | 1569 | 18.805 | -0.779 | 20.754 | 1.00 | 29.74 |
| ATOM | 933 | O | LEU | 1569 | 19.530 | -1.484 | 21.447 | 1.00 | 28.35 |
| ATOM | 934 | N | ARG | 1570 | 19.179 | 0.427 | 20.341 | 1.00 | 31.42 |
| ATOM | 936 | CA | ARG | 1570 | 20.485 | 0.985 | 20.703 | 1.00 | 32.81 |
| ATOM | 937 | CB | ARG | 1570 | 20.639 | 2.395 | 20.115 | 1.00 | 31.01 |
| ATOM | 938 | CG | ARG | 1570 | 21.922 | 3.091 | 20.543 | 1.00 | 35.33 |
| ATOM | 939 | CD | ARG | 1570 | 21.918 | 4.581 | 20.212 | 1.00 | 38.30 |
| ATOM | 940 | NE | ARG | 1570 | 20.700 | 5.272 | 20.649 | 1.00 | 47.77 |
| ATOM | 942 | CZ | ARG | 1570 | 20.393 | 5.595 | 21.912 | 1.00 | 53.56 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 943 | NH1 | ARG | 1570 | 21.212 | 5.304 | 22.931 | 1.00 | 51.30 |
| ATOM | 946 | NH2 | ARG | 1570 | 19.245 | 6.223 | 22.161 | 1.00 | 51.34 |
| ATOM | 949 | C | ARG | 1570 | 20.620 | 1.034 | 22.230 | 1.00 | 35.61 |
| ATOM | 950 | O | ARG | 1570 | 21.548 | 0.455 | 22.814 | 1.00 | 34.40 |
| ATOM | 951 | N | GLU | 1571 | 19.677 | 1.724 | 22.863 | 1.00 | 36.79 |
| ATOM | 953 | CA | GLU | 1571 | 19.637 | 1.855 | 24.311 | 1.00 | 37.35 |
| ATOM | 954 | CB | GLU | 1571 | 18.403 | 2.662 | 24.725 | 1.00 | 41.36 |
| ATOM | 955 | CG | GLU | 1571 | 18.407 | 4.118 | 24.267 | 1.00 | 49.97 |
| ATOM | 956 | CD | GLU | 1571 | 17.048 | 4.823 | 24.459 | 1.00 | 59.14 |
| ATOM | 957 | OE1 | GLU | 1571 | 15.991 | 4.133 | 24.595 | 1.00 | 59.21 |
| ATOM | 958 | OE2 | GLU | 1571 | 17.043 | 6.081 | 24.446 | 1.00 | 59.41 |
| ATOM | 959 | C | GLU | 1571 | 19.593 | 0.459 | 24.948 | 1.00 | 37.09 |
| ATOM | 960 | O | GLU | 1571 | 20.327 | 0.172 | 25.892 | 1.00 | 37.70 |
| ATOM | 961 | N | TYR | 1572 | 18.750 | -0.405 | 24.400 | 1.00 | 35.08 |
| ATOM | 963 | CA | TYR | 1572 | 18.591 | -1.766 | 24.878 | 1.00 | 32.72 |
| ATOM | 964 | CB | TYR | 1572 | 17.571 | -2.499 | 23.995 | 1.00 | 31.62 |
| ATOM | 965 | CG | TYR | 1572 | 17.376 | -3.973 | 24.309 | 1.00 | 25.69 |
| ATOM | 966 | CD1 | TYR | 1572 | 16.392 | -4.378 | 25.187 | 1.00 | 27.87 |
| ATOM | 967 | CE1 | TYR | 1572 | 16.180 | -5.711 | 25.458 | 1.00 | 28.57 |
| ATOM | 968 | CD2 | TYR | 1572 | 18.151 | -4.941 | 23.703 | 1.00 | 22.18 |
| ATOM | 969 | CE2 | TYR | 1572 | 17.948 | -6.284 | 23.969 | 1.00 | 25.06 |
| ATOM | 970 | CZ | TYR | 1572 | 16.954 | -6.659 | 24.852 | 1.00 | 25.65 |
| ATOM | 971 | OH | TYR | 1572 | 16.732 | -7.985 | 25.143 | 1.00 | 25.29 |
| ATOM | 973 | C | TYR | 1572 | 19.904 | -2.525 | 24.871 | 1.00 | 34.57 |
| ATOM | 974 | O | TYR | 1572 | 20.186 | -3.309 | 25.796 | 1.00 | 35.05 |
| ATOM | 975 | N | LEU | 1573 | 20.692 | -2.338 | 23.812 | 1.00 | 33.34 |
| ATOM | 977 | CA | LEU | 1573 | 21.970 | -3.033 | 23.712 | 1.00 | 33.00 |
| ATOM | 978 | CB | LEU | 1573 | 22.487 | -3.018 | 22.273 | 1.00 | 29.86 |
| ATOM | 979 | CG | LEU | 1573 | 21.833 | -3.888 | 21.198 | 1.00 | 23.37 |
| ATOM | 980 | CD1 | LEU | 1573 | 22.339 | -3.448 | 19.840 | 1.00 | 16.57 |
| ATOM | 981 | CD2 | LEU | 1573 | 22.129 | -5.354 | 21.426 | 1.00 | 20.31 |
| ATOM | 982 | C | LEU | 1573 | 22.997 | -2.417 | 24.655 | 1.00 | 36.57 |
| ATOM | 983 | O | LEU | 1573 | 23.752 | -3.134 | 25.311 | 1.00 | 39.00 |
| ATOM | 984 | N | GLN | 1574 | 23.003 | -1.090 | 24.735 | 1.00 | 37.26 |
| ATOM | 986 | CA | GLN | 1574 | 23.942 | -0.399 | 25.608 | 1.00 | 37.50 |
| ATOM | 987 | CB | GLN | 1574 | 23.844 | 1.110 | 25.394 | 1.00 | 36.96 |
| ATOM | 988 | CG | GLN | 1574 | 24.526 | 1.582 | 24.113 | 1.00 | 39.10 |
| ATOM | 989 | CD | GLN | 1574 | 24.289 | 3.054 | 23.801 | 1.00 | 40.63 |
| ATOM | 990 | OE1 | GLN | 1574 | 23.697 | 3.796 | 24.595 | 1.00 | 38.68 |
| ATOM | 991 | NE2 | GLN | 1574 | 24.736 | 3.480 | 22.625 | 1.00 | 38.62 |
| ATOM | 994 | C | GLN | 1574 | 23.687 | -0.759 | 27.073 | 1.00 | 38.27 |
| ATOM | 995 | O | GLN | 1574 | 24.600 | -1.144 | 27.801 | 1.00 | 39.43 |
| ATOM | 996 | N | ALA | 1575 | 22.422 | -0.731 | 27.469 | 1.00 | 38.80 |
| ATOM | 998 | CA | ALA | 1575 | 22.021 | -1.044 | 28.831 | 1.00 | 39.51 |
| ATOM | 999 | CB | ALA | 1575 | 20.551 | -0.714 | 29.024 | 1.00 | 36.89 |
| ATOM | 1000 | C | ALA | 1575 | 22.304 | -2.484 | 29.275 | 1.00 | 40.89 |
| ATOM | 1001 | O | ALA | 1575 | 22.006 | -2.842 | 30.417 | 1.00 | 44.53 |
| ATOM | 1002 | N | ARG | 1576 | 22.857 | -3.317 | 28.395 | 1.00 | 39.11 |
| ATOM | 1004 | CA | ARG | 1576 | 23.148 | -4.703 | 28.768 | 1.00 | 38.24 |
| ATOM | 1005 | CB | ARG | 1576 | 22.234 | -5.669 | 28.019 | 1.00 | 38.42 |
| ATOM | 1006 | CG | ARG | 1576 | 20.794 | -5.518 | 28.472 | 1.00 | 39.73 |
| ATOM | 1007 | CD | ARG | 1576 | 19.838 | -6.352 | 27.687 | 1.00 | 37.87 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1008 | NE | ARG | 1576 | 18.489 | -6.260 | 28.235 | 1.00 | 41.03 |
| ATOM | 1010 | CZ | ARG | 1576 | 17.830 | -5.123 | 28.436 | 1.00 | 43.27 |
| ATOM | 1011 | NH1 | ARG | 1576 | 18.399 | -3.961 | 28.143 | 1.00 | 42.64 |
| ATOM | 1014 | NH2 | ARG | 1576 | 16.573 | -5.152 | 28.877 | 1.00 | 46.13 |
| ATOM | 1017 | C | ARG | 1576 | 24.604 | -5.076 | 28.612 | 1.00 | 39.77 |
| ATOM | 1018 | O | ARG | 1576 | 24.978 | -6.256 | 28.623 | 1.00 | 40.25 |
| ATOM | 1019 | N | ARG | 1577 | 25.428 | -4.042 | 28.501 | 1.00 | 40.39 |
| ATOM | 1021 | CA | ARG | 1577 | 26.866 | -4.194 | 28.388 | 1.00 | 40.42 |
| ATOM | 1022 | CB | ARG | 1577 | 27.485 | -2.871 | 27.952 | 1.00 | 37.67 |
| ATOM | 1023 | CG | ARG | 1577 | 27.247 | -2.477 | 26.526 | 1.00 | 36.22 |
| ATOM | 1024 | CD | ARG | 1577 | 27.857 | -1.113 | 26.287 | 1.00 | 35.55 |
| ATOM | 1025 | NE | ARG | 1577 | 27.971 | -0.797 | 24.866 | 1.00 | 38.72 |
| ATOM | 1027 | CZ | ARG | 1577 | 28.395 | 0.369 | 24.384 | 1.00 | 37.57 |
| ATOM | 1028 | NH1 | ARG | 1577 | 28.754 | 1.352 | 25.205 | 1.00 | 37.49 |
| ATOM | 1031 | NH2 | ARG | 1577 | 28.449 | 0.562 | 23.074 | 1.00 | 39.58 |
| ATOM | 1034 | C | ARG | 1577 | 27.449 | -4.548 | 29.760 | 1.00 | 42.45 |
| ATOM | 1035 | O | ARG | 1577 | 26.878 | -4.180 | 30.801 | 1.00 | 42.57 |
| ATOM | 1036 | N | PRO | 1578 | 28.564 | -5.296 | 29.797 | 1.00 | 43.36 |
| ATOM | 1037 | CD | PRO | 1578 | 29.270 | -5.985 | 28.692 | 1.00 | 42.43 |
| ATOM | 1038 | CA | PRO | 1578 | 29.159 | -5.648 | 31.082 | 1.00 | 43.08 |
| ATOM | 1039 | CB | PRO | 1578 | 30.225 | -6.676 | 30.709 | 1.00 | 40.33 |
| ATOM | 1040 | CG | PRO | 1578 | 30.600 | -6.300 | 29.331 | 1.00 | 40.71 |
| ATOM | 1041 | C | PRO | 1578 | 29.768 | -4.373 | 31.666 | 1.00 | 42.44 |
| ATOM | 1042 | O | PRO | 1578 | 30.261 | -3.525 | 30.922 | 1.00 | 41.24 |
| ATOM | 1043 | N | PRO | 1579 | 29.705 | -4.205 | 32.993 | 1.00 | 44.57 |
| ATOM | 1044 | CD | PRO | 1579 | 29.169 | -5.143 | 33.994 | 1.00 | 46.68 |
| ATOM | 1045 | CA | PRO | 1579 | 30.251 | -3.017 | 33.654 | 1.00 | 44.89 |
| ATOM | 1046 | CB | PRO | 1579 | 30.088 | -3.356 | 35.134 | 1.00 | 45.31 |
| ATOM | 1047 | CG | PRO | 1579 | 28.865 | -4.224 | 35.142 | 1.00 | 44.45 |
| ATOM | 1048 | C | PRO | 1579 | 31.711 | -2.767 | 33.289 | 1.00 | 45.17 |
| ATOM | 1049 | O | PRO | 1579 | 32.620 | -3.257 | 33.953 | 1.00 | 47.72 |
| ATOM | 1050 | N | ALA | 1592 | 19.075 | -5.384 | 32.475 | 1.00 | 49.23 |
| ATOM | 1052 | CA | ALA | 1592 | 20.500 | -5.078 | 32.354 | 1.00 | 50.33 |
| ATOM | 1053 | CB | ALA | 1592 | 20.954 | -4.184 | 33.503 | 1.00 | 51.83 |
| ATOM | 1054 | C | ALA | 1592 | 21.412 | -6.308 | 32.251 | 1.00 | 50.65 |
| ATOM | 1055 | O | ALA | 1592 | 22.621 | -6.166 | 32.044 | 1.00 | 51.55 |
| ATOM | 1056 | N | ALA | 1593 | 20.849 | -7.505 | 32.409 | 1.00 | 49.06 |
| ATOM | 1058 | CA | ALA | 1593 | 21.638 | -8.735 | 32.294 | 1.00 | 48.07 |
| ATOM | 1059 | CB | ALA | 1593 | 20.773 | -9.953 | 32.579 | 1.00 | 47.87 |
| ATOM | 1060 | C | ALA | 1593 | 22.258 | -8.840 | 30.891 | 1.00 | 47.59 |
| ATOM | 1061 | O | ALA | 1593 | 21.664 | -8.426 | 29.894 | 1.00 | 49.09 |
| ATOM | 1062 | N | GLN | 1594 | 23.465 | -9.388 | 30.830 | 1.00 | 47.30 |
| ATOM | 1064 | CA | GLN | 1594 | 24.186 | -9.553 | 29.569 | 1.00 | 45.32 |
| ATOM | 1065 | CB | GLN | 1594 | 25.576 | -10.118 | 29.837 | 1.00 | 44.82 |
| ATOM | 1066 | CG | GLN | 1594 | 26.523 | -9.166 | 30.542 | 1.00 | 49.34 |
| ATOM | 1067 | CD | GLN | 1594 | 27.751 | -9.877 | 31.111 | 1.00 | 52.40 |
| ATOM | 1068 | OE1 | GLN | 1594 | 28.264 | -10.847 | 30.537 | 1.00 | 51.16 |
| ATOM | 1069 | NE2 | GLN | 1594 | 28.209 | -9.408 | 32.265 | 1.00 | 54.00 |
| ATOM | 1072 | C | GLN | 1594 | 23.474 | -10.432 | 28.539 | 1.00 | 45.00 |
| ATOM | 1073 | O | GLN | 1594 | 22.780 | -11.393 | 28.876 | 1.00 | 45.28 |
| ATOM | 1074 | N | LEU | 1595 | 23.684 | -10.104 | 27.273 | 1.00 | 45.08 |
| ATOM | 1076 | CA | LEU | 1595 | 23.084 | -10.828 | 26.169 | 1.00 | 44.65 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1077 | CB | LEU | 1595 | 22.758 | -9.864 | 25.023 | 1.00 | 43.08 |
| ATOM | 1078 | CG | LEU | 1595 | 21.619 | -8.877 | 25.295 | 1.00 | 43.22 |
| ATOM | 1079 | CD1 | LEU | 1595 | 21.855 | -7.563 | 24.564 | 1.00 | 41.25 |
| ATOM | 1080 | CD2 | LEU | 1595 | 20.276 | -9.510 | 24.918 | 1.00 | 41.96 |
| ATOM | 1081 | C | LEU | 1595 | 24.044 | -11.885 | 25.685 | 1.00 | 44.58 |
| ATOM | 1082 | O | LEU | 1595 | 25.252 | -11.661 | 25.632 | 1.00 | 44.62 |
| ATOM | 1083 | N | SER | 1596 | 23.511 | -13.058 | 25.376 | 1.00 | 45.71 |
| ATOM | 1085 | CA | SER | 1596 | 24.325 | -14.151 | 24.868 | 1.00 | 45.30 |
| ATOM | 1086 | CB | SER | 1596 | 23.633 | -15.495 | 25.124 | 1.00 | 46.19 |
| ATOM | 1087 | OG | SER | 1596 | 22.401 | -15.605 | 24.432 | 1.00 | 44.03 |
| ATOM | 1089 | C | SER | 1596 | 24.557 | -13.968 | 23.366 | 1.00 | 45.09 |
| ATOM | 1090 | O | SER | 1596 | 23.891 | -13.156 | 22.707 | 1.00 | 45.03 |
| ATOM | 1091 | N | SER | 1597 | 25.475 | -14.756 | 22.823 | 1.00 | 44.55 |
| ATOM | 1093 | CA | SER | 1597 | 25.782 | -14.690 | 21.407 | 1.00 | 45.00 |
| ATOM | 1094 | CB | SER | 1597 | 26.921 | -15.643 | 21.065 | 1.00 | 45.60 |
| ATOM | 1095 | OG | SER | 1597 | 27.976 | -15.516 | 22.007 | 1.00 | 54.80 |
| ATOM | 1097 | C | SER | 1597 | 24.526 | -15.076 | 20.633 | 1.00 | 43.92 |
| ATOM | 1098 | O | SER | 1597 | 24.233 | -14.498 | 19.577 | 1.00 | 45.51 |
| ATOM | 1099 | N | LYS | 1598 | 23.767 | -16.025 | 21.178 | 1.00 | 39.36 |
| ATOM | 1101 | CA | LYS | 1598 | 22.551 | -16.454 | 20.519 | 1.00 | 36.56 |
| ATOM | 1102 | CB | LYS | 1598 | 21.978 | -17.715 | 21.147 | 1.00 | 34.93 |
| ATOM | 1103 | CG | LYS | 1598 | 21.374 | -18.643 | 20.101 | 1.00 | 37.52 |
| ATOM | 1104 | CD | LYS | 1598 | 20.450 | -19.665 | 20.706 | 1.00 | 34.85 |
| ATOM | 1105 | CE | LYS | 1598 | 20.054 | -20.709 | 19.702 | 1.00 | 30.95 |
| ATOM | 1106 | NZ | LYS | 1598 | 21.219 | -21.551 | 19.334 | 1.00 | 30.59 |
| ATOM | 1110 | C | LYS | 1598 | 21.521 | -15.336 | 20.552 | 1.00 | 36.21 |
| ATOM | 1111 | O | LYS | 1598 | 20.840 | -15.099 | 19.548 | 1.00 | 36.39 |
| ATOM | 1112 | N | ASP | 1599 | 21.447 | -14.624 | 21.681 | 1.00 | 33.57 |
| ATOM | 1114 | CA | ASP | 1599 | 20.520 | -13.508 | 21.841 | 1.00 | 31.94 |
| ATOM | 1115 | CB | ASP | 1599 | 20.635 | -12.898 | 23.238 | 1.00 | 33.82 |
| ATOM | 1116 | CG | ASP | 1599 | 20.143 | -13.838 | 24.339 | 1.00 | 38.08 |
| ATOM | 1117 | OD1 | ASP | 1599 | 20.659 | -13.717 | 25.475 | 1.00 | 37.52 |
| ATOM | 1118 | OD2 | ASP | 1599 | 19.256 | -14.691 | 24.072 | 1.00 | 36.17 |
| ATOM | 1119 | C | ASP | 1599 | 20.777 | -12.430 | 20.802 | 1.00 | 30.89 |
| ATOM | 1120 | O | ASP | 1599 | 19.846 | -11.945 | 20.153 | 1.00 | 30.88 |
| ATOM | 1121 | N | LEU | 1600 | 22.046 | -12.070 | 20.636 | 1.00 | 31.39 |
| ATOM | 1123 | CA | LEU | 1600 | 22.439 | -11.050 | 19.666 | 1.00 | 31.55 |
| ATOM | 1124 | CB | LEU | 1600 | 23.921 | -10.695 | 19.845 | 1.00 | 30.47 |
| ATOM | 1125 | CG | LEU | 1600 | 24.341 | -10.072 | 21.190 | 1.00 | 29.24 |
| ATOM | 1126 | CD1 | LEU | 1600 | 25.857 | -9.923 | 21.226 | 1.00 | 29.75 |
| ATOM | 1127 | CD2 | LEU | 1600 | 23.666 | -8.731 | 21.404 | 1.00 | 24.50 |
| ATOM | 1128 | C | LEU | 1600 | 22.136 | -11.478 | 18.212 | 1.00 | 31.39 |
| ATOM | 1129 | O | LEU | 1600 | 21.620 | -10.686 | 17.418 | 1.00 | 31.23 |
| ATOM | 1130 | N | VAL | 1601 | 22.439 | -12.729 | 17.863 | 1.00 | 30.00 |
| ATOM | 1132 | CA | VAL | 1601 | 22.161 | -13.231 | 16.518 | 1.00 | 27.94 |
| ATOM | 1133 | CB | VAL | 1601 | 22.827 | -14.600 | 16.261 | 1.00 | 27.68 |
| ATOM | 1134 | CG1 | VAL | 1601 | 22.467 | -15.108 | 14.885 | 1.00 | 24.69 |
| ATOM | 1135 | CG2 | VAL | 1601 | 24.326 | -14.474 | 16.362 | 1.00 | 25.87 |
| ATOM | 1136 | C | VAL | 1601 | 20.642 | -13.340 | 16.310 | 1.00 | 28.98 |
| ATOM | 1137 | O | VAL | 1601 | 20.152 | -13.151 | 15.191 | 1.00 | 28.55 |
| ATOM | 1138 | N | SER | 1602 | 19.904 | -13.635 | 17.382 | 1.00 | 27.64 |
| ATOM | 1140 | CA | SER | 1602 | 18.450 | -13.726 | 17.318 | 1.00 | 27.07 |

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ATOM   1141  CB  SER  1602      17.899 -14.362  18.584  1.00 29.97
ATOM   1142  OG  SER  1602      16.488 -14.202  18.673  1.00 38.86
ATOM   1144  C   SER  1602      17.864 -12.327  17.093  1.00 27.45
ATOM   1145  O   SER  1602      16.826 -12.181  16.438  1.00 29.38
ATOM   1146  N   CYS  1603      18.504 -11.306  17.663  1.00 25.31
ATOM   1148  CA  CYS  1603      18.087  -9.909  17.461  1.00 24.49
ATOM   1149  CB  CYS  1603      19.074  -8.965  18.143  1.00 21.15
ATOM   1150  SG  CYS  1603      18.716  -7.213  18.030  0.50 11.83 PRT1
ATOM   1151  C   CYS  1603      18.155  -9.628  15.961  1.00 26.92
ATOM   1152  O   CYS  1603      17.175  -9.238  15.329  1.00 30.04
ATOM   1153  N   ALA  1604      19.340  -9.833  15.398  1.00 28.35
ATOM   1155  CA  ALA  1604      19.573  -9.611  13.979  1.00 28.00
ATOM   1156  CB  ALA  1604      20.970 -10.098  13.588  1.00 25.49
ATOM   1157  C   ALA  1604      18.517 -10.295  13.132  1.00 26.69
ATOM   1158  O   ALA  1604      17.892  -9.646  12.310  1.00 31.40
ATOM   1159  N   TYR  1605      18.270 -11.577  13.399  1.00 26.33
ATOM   1161  CA  TYR  1605      17.286 -12.384  12.666  1.00 24.79
ATOM   1162  CB  TYR  1605      17.209 -13.771  13.300  1.00 23.42
ATOM   1163  CG  TYR  1605      16.132 -14.663  12.742  1.00 29.93
ATOM   1164  CD1 TYR  1605      16.281 -15.298  11.510  1.00 30.00
ATOM   1165  CE1 TYR  1605      15.270 -16.097  10.989  1.00 32.29
ATOM   1166  CD2 TYR  1605      14.949 -14.859  13.441  1.00 32.69
ATOM   1167  CE2 TYR  1605      13.935 -15.650  12.934  1.00 33.02
ATOM   1168  CZ  TYR  1605      14.091 -16.266  11.713  1.00 34.40
ATOM   1169  OH  TYR  1605      13.037 -17.023  11.225  1.00 34.18
ATOM   1171  C   TYR  1605      15.885 -11.750  12.572  1.00 26.08
ATOM   1172  O   TYR  1605      15.327 -11.587  11.475  1.00 25.43
ATOM   1173  N   GLN  1606      15.337 -11.366  13.717  1.00 25.38
ATOM   1175  CA  GLN  1606      14.018 -10.737  13.776  1.00 25.47
ATOM   1176  CB  GLN  1606      13.662 -10.424  15.227  1.00 24.21
ATOM   1177  CG  GLN  1606      13.642 -11.636  16.127  1.00 24.37
ATOM   1178  CD  GLN  1606      13.237 -11.279  17.540  1.00 27.16
ATOM   1179  OE1 GLN  1606      12.227 -10.603  17.758  1.00 29.64
ATOM   1180  NE2 GLN  1606      14.033 -11.705  18.507  1.00 30.69
ATOM   1183  C   GLN  1606      13.953  -9.449  12.949  1.00 26.89
ATOM   1184  O   GLN  1606      12.936  -9.136  12.319  1.00 26.40
ATOM   1185  N   VAL  1607      15.030  -8.674  13.000  1.00 27.79
ATOM   1187  CA  VAL  1607      15.120  -7.430  12.255  1.00 26.35
ATOM   1188  CB  VAL  1607      16.408  -6.667  12.625  1.00 24.87
ATOM   1189  CG1 VAL  1607      16.556  -5.433  11.752  1.00 25.90
ATOM   1190  CG2 VAL  1607      16.382  -6.282  14.094  1.00 17.95
ATOM   1191  C   VAL  1607      15.121  -7.743  10.757  1.00 27.69
ATOM   1192  O   VAL  1607      14.406  -7.093   9.979  1.00 30.85
ATOM   1193  N   ALA  1608      15.902  -8.749  10.355  1.00 24.59
ATOM   1195  CA  ALA  1608      15.965  -9.135   8.950  1.00 23.22
ATOM   1196  CB  ALA  1608      16.971 -10.227   8.750  1.00 17.65
ATOM   1197  C   ALA  1608      14.579  -9.589   8.492  1.00 24.58
ATOM   1198  O   ALA  1608      14.201  -9.372   7.337  1.00 26.22
ATOM   1199  N   ARG  1609      13.819 -10.191   9.409  1.00 25.65
ATOM   1201  CA  ARG  1609      12.453 -10.648   9.124  1.00 24.86
ATOM   1202  CB  ARG  1609      11.998 -11.660  10.160  1.00 28.15
ATOM   1203  CG  ARG  1609      12.451 -13.050   9.863  1.00 30.10
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1204 | CD | ARG | 1609 | 11.683 | -13.980 | 10.723 | 1.00 | 32.49 |
| ATOM | 1205 | NE | ARG | 1609 | 10.942 | -14.941 | 9.927 | 1.00 | 34.58 |
| ATOM | 1207 | CZ | ARG | 1609 | 10.058 | -15.792 | 10.437 | 1.00 | 35.69 |
| ATOM | 1208 | NH1 | ARG | 1609 | 9.800 | -15.790 | 11.740 | 1.00 | 32.47 |
| ATOM | 1211 | NH2 | ARG | 1609 | 9.468 | -16.678 | 9.645 | 1.00 | 36.67 |
| ATOM | 1214 | C | ARG | 1609 | 11.421 | -9.518 | 9.008 | 1.00 | 22.96 |
| ATOM | 1215 | O | ARG | 1609 | 10.522 | -9.582 | 8.155 | 1.00 | 23.65 |
| ATOM | 1216 | N | GLY | 1610 | 11.501 | -8.522 | 9.888 | 1.00 | 20.88 |
| ATOM | 1218 | CA | GLY | 1610 | 10.591 | -7.398 | 9.789 | 1.00 | 21.47 |
| ATOM | 1219 | C | GLY | 1610 | 10.822 | -6.741 | 8.432 | 1.00 | 23.55 |
| ATOM | 1220 | O | GLY | 1610 | 9.872 | -6.452 | 7.688 | 1.00 | 23.53 |
| ATOM | 1221 | N | MET | 1611 | 12.097 | -6.558 | 8.088 | 1.00 | 24.37 |
| ATOM | 1223 | CA | MET | 1611 | 12.488 | -5.955 | 6.809 | 1.00 | 25.10 |
| ATOM | 1224 | CB | MET | 1611 | 13.991 | -5.686 | 6.801 | 1.00 | 25.47 |
| ATOM | 1225 | CG | MET | 1611 | 14.391 | -4.478 | 7.652 | 1.00 | 27.09 |
| ATOM | 1226 | SD | MET | 1611 | 13.362 | -3.000 | 7.330 | 1.00 | 22.57 |
| ATOM | 1227 | CE | MET | 1611 | 13.665 | -2.715 | 5.612 | 1.00 | 21.91 |
| ATOM | 1228 | C | MET | 1611 | 12.090 | -6.791 | 5.590 | 1.00 | 26.57 |
| ATOM | 1229 | O | MET | 1611 | 11.700 | -6.251 | 4.553 | 1.00 | 24.98 |
| ATOM | 1230 | N | GLU | 1612 | 12.213 | -8.108 | 5.710 | 1.00 | 27.89 |
| ATOM | 1232 | CA | GLU | 1612 | 11.836 | -9.003 | 4.632 | 1.00 | 26.91 |
| ATOM | 1233 | CB | GLU | 1612 | 12.120 | -10.446 | 5.024 | 1.00 | 26.70 |
| ATOM | 1234 | CG | GLU | 1612 | 11.602 | -11.443 | 4.026 | 1.00 | 29.25 |
| ATOM | 1235 | CD | GLU | 1612 | 11.796 | -12.872 | 4.477 | 1.00 | 31.24 |
| ATOM | 1236 | OE1 | GLU | 1612 | 11.658 | -13.143 | 5.692 | 1.00 | 33.39 |
| ATOM | 1237 | OE2 | GLU | 1612 | 12.085 | -13.733 | 3.617 | 1.00 | 31.91 |
| ATOM | 1238 | C | GLU | 1612 | 10.354 | -8.812 | 4.305 | 1.00 | 27.55 |
| ATOM | 1239 | O | GLU | 1612 | 9.974 | -8.697 | 3.130 | 1.00 | 30.04 |
| ATOM | 1240 | N | TYR | 1613 | 9.518 | -8.752 | 5.337 | 1.00 | 25.13 |
| ATOM | 1242 | CA | TYR | 1613 | 8.092 | -8.545 | 5.133 | 1.00 | 21.91 |
| ATOM | 1243 | CB | TYR | 1613 | 7.341 | -8.625 | 6.462 | 1.00 | 21.00 |
| ATOM | 1244 | CG | TYR | 1613 | 5.867 | -8.318 | 6.335 | 1.00 | 17.47 |
| ATOM | 1245 | CD1 | TYR | 1613 | 4.969 | -9.307 | 5.968 | 1.00 | 18.34 |
| ATOM | 1246 | CE1 | TYR | 1613 | 3.610 | -9.049 | 5.872 | 1.00 | 18.83 |
| ATOM | 1247 | CD2 | TYR | 1613 | 5.373 | -7.041 | 6.600 | 1.00 | 14.48 |
| ATOM | 1248 | CE2 | TYR | 1613 | 4.017 | -6.761 | 6.502 | 1.00 | 19.67 |
| ATOM | 1249 | CZ | TYR | 1613 | 3.137 | -7.776 | 6.135 | 1.00 | 22.67 |
| ATOM | 1250 | OH | TYR | 1613 | 1.779 | -7.542 | 6.009 | 1.00 | 21.91 |
| ATOM | 1252 | C | TYR | 1613 | 7.870 | -7.170 | 4.504 | 1.00 | 22.06 |
| ATOM | 1253 | O | TYR | 1613 | 7.125 | -7.034 | 3.540 | 1.00 | 22.01 |
| ATOM | 1254 | N | LEU | 1614 | 8.541 | -6.154 | 5.045 | 1.00 | 22.04 |
| ATOM | 1256 | CA | LEU | 1614 | 8.400 | -4.794 | 4.536 | 1.00 | 20.56 |
| ATOM | 1257 | CB | LEU | 1614 | 9.219 | -3.830 | 5.392 | 1.00 | 18.43 |
| ATOM | 1258 | CG | LEU | 1614 | 8.548 | -3.413 | 6.707 | 1.00 | 15.96 |
| ATOM | 1259 | CD1 | LEU | 1614 | 9.509 | -2.571 | 7.518 | 1.00 | 15.70 |
| ATOM | 1260 | CD2 | LEU | 1614 | 7.255 | -2.647 | 6.436 | 1.00 | 11.06 |
| ATOM | 1261 | C | LEU | 1614 | 8.793 | -4.671 | 3.066 | 1.00 | 22.69 |
| ATOM | 1262 | O | LEU | 1614 | 8.156 | -3.939 | 2.294 | 1.00 | 24.91 |
| ATOM | 1263 | N | ALA | 1615 | 9.840 | -5.397 | 2.684 | 1.00 | 24.55 |
| ATOM | 1265 | CA | ALA | 1615 | 10.333 | -5.408 | 1.317 | 1.00 | 21.18 |
| ATOM | 1266 | CB | ALA | 1615 | 11.685 | -6.088 | 1.254 | 1.00 | 18.35 |
| ATOM | 1267 | C | ALA | 1615 | 9.334 | -6.107 | 0.404 | 1.00 | 21.97 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1268 | O | ALA | 1615 | 9.089 | -5.642 | -0.705 | 1.00 | 23.80 |
| ATOM | 1269 | N | SER | 1616 | 8.704 | -7.173 | 0.893 | 1.00 | 22.49 |
| ATOM | 1271 | CA | SER | 1616 | 7.722 | -7.919 | 0.097 | 1.00 | 21.81 |
| ATOM | 1272 | CB | SER | 1616 | 7.305 | -9.179 | 0.831 | 1.00 | 19.78 |
| ATOM | 1273 | OG | SER | 1616 | 6.382 | -8.862 | 1.851 | 1.00 | 23.88 |
| ATOM | 1275 | C | SER | 1616 | 6.475 | -7.071 | -0.149 | 1.00 | 23.60 |
| ATOM | 1276 | O | SER | 1616 | 5.733 | -7.277 | -1.117 | 1.00 | 21.74 |
| ATOM | 1277 | N | LYS | 1617 | 6.217 | -6.169 | 0.789 | 1.00 | 25.84 |
| ATOM | 1279 | CA | LYS | 1617 | 5.078 | -5.280 | 0.705 | 1.00 | 23.96 |
| ATOM | 1280 | CB | LYS | 1617 | 4.555 | -4.951 | 2.099 | 1.00 | 20.74 |
| ATOM | 1281 | CG | LYS | 1617 | 3.843 | -6.124 | 2.750 | 1.00 | 23.40 |
| ATOM | 1282 | CD | LYS | 1617 | 2.509 | -6.395 | 2.081 | 1.00 | 28.70 |
| ATOM | 1283 | CE | LYS | 1617 | 1.714 | -7.442 | 2.809 | 1.00 | 31.16 |
| ATOM | 1284 | NZ | LYS | 1617 | 2.339 | -8.767 | 2.616 | 1.00 | 41.91 |
| ATOM | 1288 | C | LYS | 1617 | 5.409 | -4.019 | -0.061 | 1.00 | 24.25 |
| ATOM | 1289 | O | LYS | 1617 | 4.640 | -3.053 | -0.022 | 1.00 | 25.22 |
| ATOM | 1290 | N | LYS | 1618 | 6.557 | -4.028 | -0.748 | 1.00 | 24.20 |
| ATOM | 1292 | CA | LYS | 1618 | 7.014 | -2.904 | -1.582 | 1.00 | 25.15 |
| ATOM | 1293 | CB | LYS | 1618 | 5.906 | -2.507 | -2.571 | 1.00 | 27.00 |
| ATOM | 1294 | CG | LYS | 1618 | 5.735 | -3.411 | -3.790 | 1.00 | 29.09 |
| ATOM | 1295 | CD | LYS | 1618 | 5.506 | -4.864 | -3.432 | 1.00 | 31.82 |
| ATOM | 1296 | CE | LYS | 1618 | 5.533 | -5.752 | -4.663 | 1.00 | 30.21 |
| ATOM | 1297 | NZ | LYS | 1618 | 4.231 | -5.707 | -5.369 | 1.00 | 26.34 |
| ATOM | 1301 | C | LYS | 1618 | 7.466 | -1.658 | -0.816 | 1.00 | 23.50 |
| ATOM | 1302 | O | LYS | 1618 | 7.537 | -0.576 | -1.385 | 1.00 | 22.10 |
| ATOM | 1303 | N | CYS | 1619 | 7.827 | -1.821 | 0.449 | 1.00 | 23.72 |
| ATOM | 1305 | CA | CYS | 1619 | 8.213 | -0.693 | 1.276 | 1.00 | 20.89 |
| ATOM | 1306 | CB | CYS | 1619 | 7.535 | -0.814 | 2.647 | 1.00 | 18.41 |
| ATOM | 1307 | SG | CYS | 1619 | 8.019 | 0.405 | 3.894 | 1.00 | 26.34 |
| ATOM | 1308 | C | CYS | 1619 | 9.717 | -0.529 | 1.451 | 1.00 | 22.94 |
| ATOM | 1309 | O | CYS | 1619 | 10.419 | -1.487 | 1.790 | 1.00 | 23.20 |
| ATOM | 1310 | N | ILE | 1620 | 10.197 | 0.690 | 1.211 | 1.00 | 21.17 |
| ATOM | 1312 | CA | ILE | 1620 | 11.610 | 1.039 | 1.388 | 1.00 | 22.35 |
| ATOM | 1313 | CB | ILE | 1620 | 12.151 | 1.823 | 0.172 | 1.00 | 17.30 |
| ATOM | 1314 | CG2 | ILE | 1620 | 13.607 | 2.215 | 0.393 | 1.00 | 8.27 |
| ATOM | 1315 | CG1 | ILE | 1620 | 11.966 | 0.997 | -1.111 | 1.00 | 18.27 |
| ATOM | 1316 | CD1 | ILE | 1620 | 12.127 | 1.803 | -2.401 | 1.00 | 17.57 |
| ATOM | 1317 | C | ILE | 1620 | 11.631 | 1.926 | 2.652 | 1.00 | 25.20 |
| ATOM | 1318 | O | ILE | 1620 | 10.912 | 2.932 | 2.715 | 1.00 | 29.69 |
| ATOM | 1319 | N | HIS | 1621 | 12.398 | 1.526 | 3.665 | 1.00 | 22.66 |
| ATOM | 1321 | CA | HIS | 1621 | 12.463 | 2.254 | 4.931 | 1.00 | 22.78 |
| ATOM | 1322 | CB | HIS | 1621 | 13.214 | 1.425 | 5.980 | 1.00 | 22.65 |
| ATOM | 1323 | CG | HIS | 1621 | 13.024 | 1.897 | 7.398 | 1.00 | 22.07 |
| ATOM | 1324 | CD2 | HIS | 1621 | 12.485 | 1.280 | 8.475 | 1.00 | 20.50 |
| ATOM | 1325 | ND1 | HIS | 1621 | 13.449 | 3.134 | 7.842 | 1.00 | 23.11 |
| ATOM | 1327 | CE1 | HIS | 1621 | 13.182 | 3.253 | 9.131 | 1.00 | 23.92 |
| ATOM | 1328 | NE2 | HIS | 1621 | 12.596 | 2.144 | 9.543 | 1.00 | 24.44 |
| ATOM | 1330 | C | HIS | 1621 | 13.110 | 3.616 | 4.831 | 1.00 | 24.07 |
| ATOM | 1331 | O | HIS | 1621 | 12.561 | 4.597 | 5.306 | 1.00 | 24.37 |
| ATOM | 1332 | N | ARG | 1622 | 14.327 | 3.639 | 4.291 | 1.00 | 26.42 |
| ATOM | 1334 | CA | ARG | 1622 | 15.129 | 4.853 | 4.130 | 1.00 | 24.59 |
| ATOM | 1335 | CB | ARG | 1622 | 14.289 | 6.018 | 3.581 | 1.00 | 17.58 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1336 | CG | ARG | 1622 | 13.810 | 5.767 | 2.163 | 1.00 | 13.88 |
| ATOM | 1337 | CD | ARG | 1622 | 12.925 | 6.860 | 1.634 | 0.50 | 4.97 |
| ATOM | 1338 | NE | ARG | 1622 | 12.574 | 6.590 | 0.243 | 0.50 | 6.49 |
| ATOM | 1340 | CZ | ARG | 1622 | 11.537 | 5.852 | -0.145 | 0.50 | 3.84 |
| ATOM | 1341 | NH1 | ARG | 1622 | 10.719 | 5.308 | 0.753 | 0.50 | 2.25 |
| ATOM | 1344 | NH2 | ARG | 1622 | 11.356 | 5.611 | -1.433 | 0.50 | 2.48 |
| ATOM | 1347 | C | ARG | 1622 | 15.918 | 5.257 | 5.388 | 1.00 | 24.72 |
| ATOM | 1348 | O | ARG | 1622 | 16.767 | 6.138 | 5.337 | 1.00 | 26.90 |
| ATOM | 1349 | N | ASP | 1623 | 15.685 | 4.585 | 6.505 | 1.00 | 25.61 |
| ATOM | 1351 | CA | ASP | 1623 | 16.437 | 4.927 | 7.703 | 1.00 | 28.41 |
| ATOM | 1352 | CB | ASP | 1623 | 15.922 | 6.213 | 8.349 | 1.00 | 30.38 |
| ATOM | 1353 | CG | ASP | 1623 | 16.891 | 6.772 | 9.373 | 1.00 | 33.47 |
| ATOM | 1354 | OD1 | ASP | 1623 | 16.428 | 7.338 | 10.382 | 1.00 | 43.35 |
| ATOM | 1355 | OD2 | ASP | 1623 | 18.121 | 6.645 | 9.167 | 1.00 | 31.88 |
| ATOM | 1356 | C | ASP | 1623 | 16.498 | 3.797 | 8.713 | 1.00 | 28.86 |
| ATOM | 1357 | O | ASP | 1623 | 16.148 | 3.959 | 9.887 | 1.00 | 28.31 |
| ATOM | 1358 | N | LEU | 1624 | 16.956 | 2.642 | 8.246 | 1.00 | 27.81 |
| ATOM | 1360 | CA | LEU | 1624 | 17.087 | 1.480 | 9.107 | 1.00 | 27.28 |
| ATOM | 1361 | CB | LEU | 1624 | 17.149 | 0.220 | 8.242 | 1.00 | 27.53 |
| ATOM | 1362 | CG | LEU | 1624 | 17.118 | -1.150 | 8.916 | 1.00 | 27.69 |
| ATOM | 1363 | CD1 | LEU | 1624 | 15.850 | -1.348 | 9.756 | 1.00 | 23.77 |
| ATOM | 1364 | CD2 | LEU | 1624 | 17.228 | -2.175 | 7.805 | 1.00 | 29.15 |
| ATOM | 1365 | C | LEU | 1624 | 18.340 | 1.628 | 10.002 | 1.00 | 26.27 |
| ATOM | 1366 | O | LEU | 1624 | 19.464 | 1.773 | 9.514 | 1.00 | 25.89 |
| ATOM | 1367 | N | ALA | 1625 | 18.116 | 1.598 | 11.313 | 1.00 | 23.29 |
| ATOM | 1369 | CA | ALA | 1625 | 19.164 | 1.750 | 12.314 | 1.00 | 19.68 |
| ATOM | 1370 | CB | ALA | 1625 | 19.520 | 3.233 | 12.473 | 1.00 | 18.85 |
| ATOM | 1371 | C | ALA | 1625 | 18.575 | 1.214 | 13.613 | 1.00 | 20.79 |
| ATOM | 1372 | O | ALA | 1625 | 17.352 | 1.077 | 13.716 | 1.00 | 20.75 |
| ATOM | 1373 | N | ALA | 1626 | 19.429 | 0.942 | 14.605 | 1.00 | 22.03 |
| ATOM | 1375 | CA | ALA | 1626 | 18.969 | 0.408 | 15.900 | 1.00 | 23.43 |
| ATOM | 1376 | CB | ALA | 1626 | 20.139 | -0.048 | 16.764 | 1.00 | 22.46 |
| ATOM | 1377 | C | ALA | 1626 | 18.111 | 1.397 | 16.664 | 1.00 | 25.86 |
| ATOM | 1378 | O | ALA | 1626 | 17.333 | 1.006 | 17.523 | 1.00 | 29.51 |
| ATOM | 1379 | N | ARG | 1627 | 18.303 | 2.685 | 16.407 | 1.00 | 26.92 |
| ATOM | 1381 | CA | ARG | 1627 | 17.503 | 3.722 | 17.048 | 1.00 | 27.30 |
| ATOM | 1382 | CB | ARG | 1627 | 18.017 | 5.107 | 16.627 | 1.00 | 28.29 |
| ATOM | 1383 | CG | ARG | 1627 | 18.086 | 5.287 | 15.104 | 1.00 | 36.26 |
| ATOM | 1384 | CD | ARG | 1627 | 18.255 | 6.756 | 14.688 | 1.00 | 41.19 |
| ATOM | 1385 | NE | ARG | 1627 | 18.548 | 6.928 | 13.261 | 1.00 | 39.94 |
| ATOM | 1387 | CZ | ARG | 1627 | 19.779 | 6.904 | 12.749 | 1.00 | 42.33 |
| ATOM | 1388 | NH1 | ARG | 1627 | 20.826 | 6.721 | 13.539 | 1.00 | 44.75 |
| ATOM | 1391 | NH2 | ARG | 1627 | 19.976 | 7.059 | 11.450 | 1.00 | 41.50 |
| ATOM | 1394 | C | ARG | 1627 | 16.029 | 3.567 | 16.591 | 1.00 | 27.42 |
| ATOM | 1395 | O | ARG | 1627 | 15.092 | 3.897 | 17.333 | 1.00 | 26.53 |
| ATOM | 1396 | N | ASN | 1628 | 15.850 | 3.039 | 15.375 | 1.00 | 26.82 |
| ATOM | 1398 | CA | ASN | 1628 | 14.534 | 2.849 | 14.758 | 1.00 | 24.08 |
| ATOM | 1399 | CB | ASN | 1628 | 14.569 | 3.308 | 13.301 | 1.00 | 26.30 |
| ATOM | 1400 | CG | ASN | 1628 | 14.709 | 4.823 | 13.167 | 1.00 | 25.19 |
| ATOM | 1401 | OD1 | ASN | 1628 | 14.018 | 5.567 | 13.844 | 1.00 | 28.59 |
| ATOM | 1402 | ND2 | ASN | 1628 | 15.599 | 5.277 | 12.297 | 1.00 | 22.32 |
| ATOM | 1405 | C | ASN | 1628 | 13.945 | 1.440 | 14.862 | 1.00 | 24.35 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1406 | O | ASN | 1628 | 13.026 | 1.084 | 14.105 | 1.00 | 24.66 |
| ATOM | 1407 | N | VAL | 1629 | 14.473 | 0.637 | 15.785 | 1.00 | 22.35 |
| ATOM | 1409 | CA | VAL | 1629 | 13.988 | -0.718 | 16.055 | 1.00 | 20.65 |
| ATOM | 1410 | CB | VAL | 1629 | 15.077 | -1.813 | 15.822 | 1.00 | 18.07 |
| ATOM | 1411 | CG1 | VAL | 1629 | 14.612 | -3.142 | 16.398 | 1.00 | 11.84 |
| ATOM | 1412 | CG2 | VAL | 1629 | 15.378 | -1.977 | 14.346 | 1.00 | 12.65 |
| ATOM | 1413 | C | VAL | 1629 | 13.625 | -0.670 | 17.536 | 1.00 | 24.27 |
| ATOM | 1414 | O | VAL | 1629 | 14.427 | -0.237 | 18.361 | 1.00 | 25.94 |
| ATOM | 1415 | N | LEU | 1630 | 12.393 | -1.031 | 17.866 | 1.00 | 24.99 |
| ATOM | 1417 | CA | LEU | 1630 | 11.936 | -1.010 | 19.247 | 1.00 | 25.50 |
| ATOM | 1418 | CB | LEU | 1630 | 10.609 | -0.252 | 19.339 | 1.00 | 22.79 |
| ATOM | 1419 | CG | LEU | 1630 | 10.634 | 1.179 | 18.789 | 1.00 | 17.86 |
| ATOM | 1420 | CD1 | LEU | 1630 | 9.240 | 1.680 | 18.654 | 1.00 | 18.49 |
| ATOM | 1421 | CD2 | LEU | 1630 | 11.409 | 2.100 | 19.668 | 1.00 | 17.63 |
| ATOM | 1422 | C | LEU | 1630 | 11.833 | -2.434 | 19.829 | 1.00 | 28.29 |
| ATOM | 1423 | O | LEU | 1630 | 11.666 | -3.412 | 19.092 | 1.00 | 28.56 |
| ATOM | 1424 | N | VAL | 1631 | 11.933 | -2.542 | 21.150 | 1.00 | 29.46 |
| ATOM | 1426 | CA | VAL | 1631 | 11.883 | -3.831 | 21.833 | 1.00 | 29.40 |
| ATOM | 1427 | CB | VAL | 1631 | 13.222 | -4.105 | 22.553 | 1.00 | 27.48 |
| ATOM | 1428 | CG1 | VAL | 1631 | 13.210 | -5.477 | 23.233 | 1.00 | 24.53 |
| ATOM | 1429 | CG2 | VAL | 1631 | 14.376 | -3.976 | 21.576 | 1.00 | 22.55 |
| ATOM | 1430 | C | VAL | 1631 | 10.730 | -3.918 | 22.853 | 1.00 | 31.94 |
| ATOM | 1431 | O | VAL | 1631 | 10.630 | -3.102 | 23.787 | 1.00 | 33.13 |
| ATOM | 1432 | N | THR | 1632 | 9.866 | -4.911 | 22.659 | 1.00 | 32.21 |
| ATOM | 1434 | CA | THR | 1632 | 8.728 | -5.149 | 23.540 | 1.00 | 31.77 |
| ATOM | 1435 | CB | THR | 1632 | 7.674 | -6.061 | 22.874 | 1.00 | 32.38 |
| ATOM | 1436 | OG1 | THR | 1632 | 8.169 | -7.406 | 22.792 | 1.00 | 32.38 |
| ATOM | 1438 | CG2 | THR | 1632 | 7.330 | -5.554 | 21.480 | 1.00 | 28.05 |
| ATOM | 1439 | C | THR | 1632 | 9.157 | -5.810 | 24.842 | 1.00 | 30.39 |
| ATOM | 1440 | O | THR | 1632 | 10.256 | -6.320 | 24.947 | 1.00 | 30.28 |
| ATOM | 1441 | N | GLU | 1633 | 8.260 | -5.823 | 25.822 | 1.00 | 32.43 |
| ATOM | 1443 | CA | GLU | 1633 | 8.513 | -6.424 | 27.122 | 1.00 | 32.84 |
| ATOM | 1444 | CB | GLU | 1633 | 7.259 | -6.310 | 27.991 | 1.00 | 35.28 |
| ATOM | 1445 | CG | GLU | 1633 | 7.386 | -6.881 | 29.399 | 1.00 | 46.57 |
| ATOM | 1446 | CD | GLU | 1633 | 8.463 | -6.192 | 30.260 | 1.00 | 54.03 |
| ATOM | 1447 | OE1 | GLU | 1633 | 8.519 | -4.939 | 30.297 | 1.00 | 58.68 |
| ATOM | 1448 | OE2 | GLU | 1633 | 9.249 | -6.916 | 30.918 | 1.00 | 56.84 |
| ATOM | 1449 | C | GLU | 1633 | 8.914 | -7.889 | 26.986 | 1.00 | 35.14 |
| ATOM | 1450 | O | GLU | 1633 | 9.632 | -8.435 | 27.826 | 1.00 | 33.92 |
| ATOM | 1451 | N | ASP | 1634 | 8.456 | -8.526 | 25.910 | 1.00 | 38.25 |
| ATOM | 1453 | CA | ASP | 1634 | 8.768 | -9.941 | 25.677 | 1.00 | 39.22 |
| ATOM | 1454 | CB | ASP | 1634 | 7.588 | -10.639 | 24.990 | 1.00 | 44.88 |
| ATOM | 1455 | CG | ASP | 1634 | 6.258 | -10.420 | 25.725 | 1.00 | 54.17 |
| ATOM | 1456 | OD1 | ASP | 1634 | 6.064 | -11.042 | 26.799 | 1.00 | 56.33 |
| ATOM | 1457 | OD2 | ASP | 1634 | 5.412 | -9.622 | 25.236 | 1.00 | 54.47 |
| ATOM | 1458 | C | ASP | 1634 | 10.035 | -10.109 | 24.849 | 1.00 | 37.53 |
| ATOM | 1459 | O | ASP | 1634 | 10.395 | -11.225 | 24.495 | 1.00 | 36.33 |
| ATOM | 1460 | N | ASN | 1635 | 10.730 | -8.998 | 24.589 | 1.00 | 39.12 |
| ATOM | 1462 | CA | ASN | 1635 | 11.974 | -8.948 | 23.792 | 1.00 | 37.21 |
| ATOM | 1463 | CB | ASN | 1635 | 13.042 | -9.891 | 24.361 | 1.00 | 37.83 |
| ATOM | 1464 | CG | ASN | 1635 | 13.576 | -9.426 | 25.677 | 1.00 | 38.65 |
| ATOM | 1465 | OD1 | ASN | 1635 | 13.795 | -8.236 | 25.880 | 1.00 | 43.82 |

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ATOM   1466  ND2  ASN  1635
ATOM   1469  C    ASN  1635     13.768  -10.353   26.596   1.00  39.49
ATOM   1470  O    ASN  1635     11.807   -9.193   22.287   1.00  35.03
ATOM   1471  N    VAL  1636     12.649   -9.834   21.648   1.00  32.37
ATOM   1473  CA   VAL  1636     10.705   -8.700   21.736   1.00  33.30
ATOM   1474  CB   VAL  1636     10.418   -8.846   20.320   1.00  30.50
ATOM   1475  CG1  VAL  1636      8.895   -9.014   20.075   1.00  31.54
ATOM   1476  CG2  VAL  1636      8.600   -9.178   18.584   1.00  29.16
ATOM   1477  C    VAL  1636      8.384  -10.214   20.838   1.00  34.29
ATOM   1478  O    VAL  1636     10.908   -7.577   19.629   1.00  29.28
ATOM   1479  N    MET  1637     10.553   -6.463   20.037   1.00  27.08
ATOM   1481  CA   MET  1637     11.760   -7.755   18.623   1.00  27.82
ATOM   1482  CB   MET  1637     12.318   -6.634   17.874   1.00  27.09
ATOM   1483  CG   MET  1637     13.578   -7.070   17.127   1.00  27.47
ATOM   1484  SD   MET  1637     14.648   -7.697   18.010   1.00  28.35
ATOM   1485  CE   MET  1637     15.243   -6.594   19.297   1.00  30.41
ATOM   1486  C    MET  1637     15.104   -7.640   20.728   1.00  26.00
ATOM   1487  O    MET  1637     11.272   -6.200   16.868   1.00  26.01
ATOM   1488  N    LYS  1638     10.751   -7.034   16.131   1.00  26.05
ATOM   1490  CA   LYS  1638     10.983   -4.900   16.823   1.00  25.44
ATOM   1491  CB   LYS  1638      9.984   -4.349   15.906   1.00  22.01
ATOM   1492  CG   LYS  1638      8.693   -4.028   16.658   1.00  19.65
ATOM   1493  CD   LYS  1638      7.887   -5.254   17.034   1.00  21.22
ATOM   1494  CE   LYS  1638      6.666   -4.904   17.869   1.00  21.73
ATOM   1495  NZ   LYS  1638      5.776   -6.133   18.076   1.00  19.32
ATOM   1499  C    LYS  1638      4.970   -6.522   16.869   1.00  23.14
ATOM   1500  O    LYS  1638     10.477   -3.106   15.191   1.00  21.85
ATOM   1501  N    ILE  1639     10.896   -2.147   15.808   1.00  24.35
ATOM   1503  CA   ILE  1639     10.371   -3.110   13.878   1.00  24.47
ATOM   1504  CB   ILE  1639     10.803   -1.983   13.073   1.00  24.90
ATOM   1505  CG2  ILE  1639     11.090   -2.443   11.625   1.00  22.12
ATOM   1506  CG1  ILE  1639     11.413   -1.275   10.720   1.00  17.41
ATOM   1507  CD1  ILE  1639     12.256   -3.423   11.664   1.00  18.67
ATOM   1508  C    ILE  1639     12.309   -4.308   10.492   1.00  26.15
ATOM   1509  O    ILE  1639      9.772   -0.856   13.117   1.00  28.52
ATOM   1510  N    ALA  1640      8.557   -1.094   12.964   1.00  27.86
ATOM   1512  CA   ALA  1640     10.267    0.363   13.358   1.00  30.06
ATOM   1513  CB   ALA  1640      9.444    1.564   13.445   1.00  29.37
ATOM   1514  C    ALA  1640      9.627    2.211   14.812   1.00  28.25
ATOM   1515  O    ALA  1640      9.782    2.566   12.344   1.00  29.68
ATOM   1516  N    ASP  1641     10.808    2.453   11.660   1.00  30.81
ATOM   1518  CA   ASP  1641      8.892    3.536   12.154   1.00  30.35
ATOM   1519  CB   ASP  1641      9.067    4.608   11.154   1.00  30.40
ATOM   1520  CG   ASP  1641     10.309    5.454   11.454   1.00  32.89
ATOM   1521  OD1  ASP  1641     10.018    6.678   12.321   1.00  34.68
ATOM   1522  OD2  ASP  1641     10.952    7.497   12.469   1.00  35.84
ATOM   1523  C    ASP  1641      8.897    6.824   12.856   1.00  38.22
ATOM   1524  O    ASP  1641      9.102    4.162    9.705   1.00  28.91
ATOM   1525  N    PHE  1642      9.484    4.941    8.826   1.00  29.26
ATOM   1527  CA   PHE  1642      8.650    2.941    9.440   1.00  27.21
ATOM   1528  CB   PHE  1642      8.648    2.435    8.072   1.00  25.07
ATOM   1529  CG   PHE  1642      8.432    0.909    8.043   1.00  19.64
                                  7.135    0.451    8.639   1.00  16.47
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ATOM   1530  CD1 PHE  1642     5.974   0.400   7.878  1.00 21.72
ATOM   1531  CD2 PHE  1642     7.080   0.018   9.945  1.00 17.01
ATOM   1532  CE1 PHE  1642     4.781  -0.082   8.422  1.00 20.97
ATOM   1533  CE2 PHE  1642     5.892  -0.463  10.496  1.00 18.72
ATOM   1534  CZ  PHE  1642     4.743  -0.515   9.739  1.00 20.32
ATOM   1535  C   PHE  1642     7.667   3.174   7.157  1.00 25.57
ATOM   1536  O   PHE  1642     7.910   3.292   5.971  1.00 28.40
ATOM   1537  N   GLY  1643     6.585   3.718   7.707  1.00 25.69
ATOM   1539  CA  GLY  1643     5.631   4.427   6.866  1.00 24.81
ATOM   1540  C   GLY  1643     5.786   5.935   6.893  1.00 24.84
ATOM   1541  O   GLY  1643     4.922   6.684   6.436  1.00 19.20
ATOM   1542  N   LEU  1644     6.930   6.387   7.376  1.00 29.50
ATOM   1544  CA  LEU  1644     7.189   7.808   7.491  1.00 34.24
ATOM   1545  CB  LEU  1644     8.498   8.037   8.242  1.00 33.10
ATOM   1546  CG  LEU  1644     8.473   9.371   8.962  1.00 36.00
ATOM   1547  CD1 LEU  1644     7.520   9.212  10.127  1.00 41.52
ATOM   1548  CD2 LEU  1644     9.854   9.773   9.442  1.00 35.23
ATOM   1549  C   LEU  1644     7.213   8.578   6.179  1.00 37.54
ATOM   1550  O   LEU  1644     7.759   8.123   5.176  1.00 37.48
ATOM   1551  N   ALA  1645     6.577   9.744   6.203  1.00 41.66
ATOM   1553  CA  ALA  1645     6.524  10.652   5.067  1.00 43.66
ATOM   1554  CB  ALA  1645     5.309  11.563   5.202  1.00 38.13
ATOM   1555  C   ALA  1645     7.819  11.475   5.141  1.00 44.67
ATOM   1556  O   ALA  1645     8.105  12.082   6.176  1.00 47.17
ATOM   1557  N   ALA  1646     8.622  11.462   4.082  1.00 45.69
ATOM   1559  CA  ALA  1646     9.871  12.222   4.094  1.00 48.62
ATOM   1560  CB  ALA  1646    10.971  11.405   4.778  1.00 49.50
ATOM   1561  C   ALA  1646    10.338  12.661   2.712  1.00 50.98
ATOM   1562  O   ALA  1646    10.319  11.880   1.759  1.00 52.84
ATOM   1563  N   ASP  1647    10.755  13.919   2.598  1.00 53.09
ATOM   1565  CA  ASP  1647    11.253  14.419   1.322  1.00 55.06
ATOM   1566  CB  ASP  1647    10.868  15.887   1.092  1.00 56.05
ATOM   1567  CG  ASP  1647    11.084  16.342  -0.352  1.00 59.31
ATOM   1568  OD1 ASP  1647    12.070  15.928  -1.003  1.00 59.51
ATOM   1569  OD2 ASP  1647    10.265  17.150  -0.837  1.00 63.48
ATOM   1570  C   ASP  1647    12.770  14.264   1.332  1.00 55.26
ATOM   1571  O   ASP  1647    13.487  15.075   1.926  1.00 53.18
ATOM   1572  N   ILE  1648    13.235  13.198   0.684  1.00 56.66
ATOM   1574  CA  ILE  1648    14.652  12.877   0.595  1.00 57.79
ATOM   1575  CB  ILE  1648    14.890  11.624  -0.271  1.00 53.86
ATOM   1576  CG2 ILE  1648    14.133  10.443   0.326  1.00 52.14
ATOM   1577  CG1 ILE  1648    14.454  11.886  -1.718  1.00 48.24
ATOM   1578  CD1 ILE  1648    15.198  11.083  -2.751  1.00 43.97
ATOM   1579  C   ILE  1648    15.439  14.044   0.014  1.00 62.32
ATOM   1580  O   ILE  1648    16.591  14.271   0.380  1.00 64.72
ATOM   1581  N   HIS  1649    14.805  14.791  -0.884  1.00 65.72
ATOM   1583  CA  HIS  1649    15.450  15.941  -1.500  1.00 69.00
ATOM   1584  CB  HIS  1649    14.793  16.285  -2.844  1.00 70.35
ATOM   1585  CG  HIS  1649    15.123  15.332  -3.944  1.00 73.90
ATOM   1586  CD2 HIS  1649    16.257  14.628  -4.208  1.00 75.13
ATOM   1587  ND1 HIS  1649    14.239  15.006  -4.946  1.00 75.30
ATOM   1589  CE1 HIS  1649    14.798  14.148  -5.779  1.00 76.83
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ATOM  1590  NE2 HIS  1649
ATOM  1592  C   HIS  1649      16.025  13.905  -5.348  1.00 76.74
ATOM  1593  O   HIS  1649      15.419  17.150  -0.576  1.00 70.22
ATOM  1594  N   HIS  1650      15.517  18.284  -1.041  1.00 72.83
ATOM  1596  CA  HIS  1650      15.218  16.912   0.718  1.00 71.28
ATOM  1597  CB  HIS  1650      15.199  17.987   1.710  1.00 72.52
ATOM  1598  CG  HIS  1650      13.776  18.488   1.956  1.00 75.67
ATOM  1599  CD2 HIS  1650      13.272  19.401   0.882  1.00 82.16
ATOM  1600  ND1 HIS  1650      13.451  20.734   0.691  1.00 86.17
ATOM  1602  CE1 HIS  1650      12.529  18.955  -0.185  1.00 86.37
ATOM  1603  NE2 HIS  1650      12.262  19.972  -0.993  1.00 89.04
ATOM  1605  C   HIS  1650      12.814  21.058  -0.481  1.00 89.37
ATOM  1606  O   HIS  1650      15.856  17.593   3.029  1.00 71.11
ATOM  1607  N   ILE  1651      15.783  18.334   4.010  1.00 69.56
ATOM  1609  CA  ILE  1651      16.543  16.451   3.033  1.00 70.84
ATOM  1610  CB  ILE  1651      17.221  15.939   4.222  1.00 70.50
ATOM  1611  CG2 ILE  1651      17.622  14.462   4.031  1.00 71.73
ATOM  1612  CG1 ILE  1651      18.499  13.978   5.194  1.00 71.65
ATOM  1613  CD1 ILE  1651      16.359  13.604   3.890  1.00 73.10
ATOM  1614  C   ILE  1651      16.643  12.143   3.593  1.00 75.18
ATOM  1615  O   ILE  1651      18.472  16.734   4.569  1.00 69.85
ATOM  1616  N   ASP  1652      19.375  16.882   3.745  1.00 70.30
ATOM  1618  CA  ASP  1652      18.543  17.222   5.802  1.00 68.99
ATOM  1619  CB  ASP  1652      19.707  17.987   6.240  1.00 68.06
ATOM  1620  CG  ASP  1652      19.344  18.923   7.398  1.00 70.53
ATOM  1621  OD1 ASP  1652      20.512  19.790   7.843  1.00 72.86
ATOM  1622  OD2 ASP  1652      21.306  20.248   6.985  1.00 73.36
ATOM  1623  C   ASP  1652      20.646  20.034   9.060  1.00 76.01
ATOM  1624  O   ASP  1652      20.802  17.023   6.673  1.00 66.08
ATOM  1625  N   TYR  1653      20.746  16.457   7.762  1.00 64.92
ATOM  1627  CA  TYR  1653      21.802  16.856   5.814  1.00 64.14
ATOM  1628  CB  TYR  1653      22.926  15.968   6.089  1.00 63.02
ATOM  1629  CG  TYR  1653      23.852  15.906   4.875  1.00 61.29
ATOM  1630  CD1 TYR  1653      23.362  14.971   3.795  1.00 62.37
ATOM  1631  CE1 TYR  1653      24.153  14.679   2.684  1.00 61.11
ATOM  1632  CD2 TYR  1653      23.725  13.773   1.717  1.00 62.89
ATOM  1633  CE2 TYR  1653      22.121  14.335   3.910  1.00 64.11
ATOM  1634  CZ  TYR  1653      21.685  13.429   2.953  1.00 66.09
ATOM  1635  OH  TYR  1653      22.487  13.148   1.859  1.00 65.03
ATOM  1637  C   TYR  1653      22.044  12.239   0.921  1.00 65.78
ATOM  1638  O   TYR  1653      23.733  16.313   7.345  1.00 63.49
ATOM  1639  N   TYR  1654      24.403  15.453   7.912  1.00 63.39
ATOM  1641  CA  TYR  1654      23.644  17.564   7.789  1.00 64.37
ATOM  1642  CB  TYR  1654      24.379  18.013   8.963  1.00 63.95
ATOM  1643  CG  TYR  1654      24.947  19.417   8.741  1.00 60.86
ATOM  1644  CD1 TYR  1654      26.038  19.467   7.691  1.00 57.70
ATOM  1645  CE1 TYR  1654      25.736  19.698   6.353  1.00 58.03
ATOM  1646  CD2 TYR  1654      26.734  19.708   5.383  1.00 60.65
ATOM  1647  CE2 TYR  1654      27.364  19.252   8.035  1.00 56.79
ATOM  1648  CZ  TYR  1654      28.366  19.261   7.079  1.00 58.85
ATOM  1649  OH  TYR  1654      28.047  19.488   5.754  1.00 60.88
ATOM  1651  C   TYR  1654      29.048  19.485   4.806  1.00 64.23
                               23.560  17.980  10.239  1.00 65.89
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1652 | O | TYR | 1654 | 24.074 | 18.283 | 11.316 | 1.00 | 67.56 |
| ATOM | 1653 | N | LYS | 1655 | 22.297 | 17.586 | 10.135 | 1.00 | 67.36 |
| ATOM | 1655 | CA | LYS | 1655 | 21.443 | 17.527 | 11.315 | 1.00 | 69.11 |
| ATOM | 1656 | CB | LYS | 1655 | 19.972 | 17.611 | 10.915 | 1.00 | 69.86 |
| ATOM | 1657 | CG | LYS | 1655 | 19.019 | 17.651 | 12.090 | 1.00 | 71.45 |
| ATOM | 1658 | CD | LYS | 1655 | 17.607 | 17.867 | 11.603 | 1.00 | 75.40 |
| ATOM | 1659 | CE | LYS | 1655 | 16.595 | 17.393 | 12.627 | 1.00 | 78.22 |
| ATOM | 1660 | NZ | LYS | 1655 | 15.204 | 17.553 | 12.110 | 1.00 | 80.61 |
| ATOM | 1664 | C | LYS | 1655 | 21.714 | 16.242 | 12.093 | 1.00 | 69.65 |
| ATOM | 1665 | O | LYS | 1655 | 21.872 | 15.169 | 11.497 | 1.00 | 70.67 |
| ATOM | 1666 | N | LYS | 1656 | 21.766 | 16.358 | 13.419 | 1.00 | 68.19 |
| ATOM | 1668 | CA | LYS | 1656 | 22.035 | 15.212 | 14.275 | 1.00 | 68.00 |
| ATOM | 1669 | CB | LYS | 1656 | 22.983 | 15.618 | 15.403 | 1.00 | 65.53 |
| ATOM | 1670 | CG | LYS | 1656 | 24.395 | 15.895 | 14.946 | 1.00 | 62.71 |
| ATOM | 1671 | CD | LYS | 1656 | 25.280 | 16.221 | 16.138 | 1.00 | 64.38 |
| ATOM | 1672 | CE | LYS | 1656 | 26.764 | 16.031 | 15.832 | 1.00 | 63.23 |
| ATOM | 1673 | NZ | LYS | 1656 | 27.592 | 16.186 | 17.062 | 1.00 | 61.72 |
| ATOM | 1677 | C | LYS | 1656 | 20.777 | 14.560 | 14.855 | 1.00 | 68.73 |
| ATOM | 1678 | O | LYS | 1656 | 19.695 | 15.148 | 14.837 | 1.00 | 69.20 |
| ATOM | 1679 | N | THR | 1657 | 20.928 | 13.337 | 15.359 | 1.00 | 68.48 |
| ATOM | 1681 | CA | THR | 1657 | 19.821 | 12.607 | 15.960 | 1.00 | 67.93 |
| ATOM | 1682 | CB | THR | 1657 | 20.109 | 11.078 | 16.021 | 1.00 | 68.93 |
| ATOM | 1683 | OG1 | THR | 1657 | 21.295 | 10.823 | 16.787 | 1.00 | 68.72 |
| ATOM | 1685 | CG2 | THR | 1657 | 20.289 | 10.500 | 14.637 | 1.00 | 68.83 |
| ATOM | 1686 | C | THR | 1657 | 19.682 | 13.131 | 17.383 | 1.00 | 67.80 |
| ATOM | 1687 | O | THR | 1657 | 20.424 | 14.022 | 17.790 | 1.00 | 67.87 |
| ATOM | 1688 | N | ALA | 1658 | 18.753 | 12.569 | 18.148 | 1.00 | 68.95 |
| ATOM | 1690 | CA | ALA | 1658 | 18.580 | 12.992 | 19.537 | 1.00 | 70.64 |
| ATOM | 1691 | CB | ALA | 1658 | 17.391 | 12.254 | 20.173 | 1.00 | 71.19 |
| ATOM | 1692 | C | ALA | 1658 | 19.880 | 12.709 | 20.313 | 1.00 | 69.64 |
| ATOM | 1693 | O | ALA | 1658 | 20.394 | 13.566 | 21.042 | 1.00 | 70.13 |
| ATOM | 1694 | N | ASN | 1659 | 20.440 | 11.526 | 20.080 | 1.00 | 68.02 |
| ATOM | 1696 | CA | ASN | 1659 | 21.663 | 11.092 | 20.746 | 1.00 | 66.10 |
| ATOM | 1697 | CB | ASN | 1659 | 21.835 | 9.583 | 20.557 | 1.00 | 70.23 |
| ATOM | 1698 | CG | ASN | 1659 | 22.632 | 8.937 | 21.679 | 1.00 | 74.09 |
| ATOM | 1699 | OD1 | ASN | 1659 | 22.525 | 9.331 | 22.840 | 1.00 | 75.21 |
| ATOM | 1700 | ND2 | ASN | 1659 | 23.402 | 7.907 | 21.342 | 1.00 | 75.03 |
| ATOM | 1703 | C | ASN | 1659 | 22.910 | 11.816 | 20.249 | 1.00 | 63.30 |
| ATOM | 1704 | O | ASN | 1659 | 24.004 | 11.585 | 20.762 | 1.00 | 61.12 |
| ATOM | 1705 | N | GLY | 1660 | 22.744 | 12.678 | 19.246 | 1.00 | 61.61 |
| ATOM | 1707 | CA | GLY | 1660 | 23.867 | 13.421 | 18.689 | 1.00 | 59.06 |
| ATOM | 1708 | C | GLY | 1660 | 24.604 | 12.750 | 17.536 | 1.00 | 56.84 |
| ATOM | 1709 | O | GLY | 1660 | 25.726 | 13.132 | 17.196 | 1.00 | 55.69 |
| ATOM | 1710 | N | ARG | 1661 | 23.980 | 11.758 | 16.914 | 1.00 | 55.73 |
| ATOM | 1712 | CA | ARG | 1661 | 24.626 | 11.062 | 15.808 | 1.00 | 52.76 |
| ATOM | 1713 | CB | ARG | 1661 | 24.387 | 9.549 | 15.883 | 1.00 | 52.39 |
| ATOM | 1714 | CG | ARG | 1661 | 24.977 | 8.874 | 17.111 | 1.00 | 54.08 |
| ATOM | 1715 | CD | ARG | 1661 | 24.776 | 7.376 | 17.045 | 1.00 | 58.37 |
| ATOM | 1716 | NE | ARG | 1661 | 25.178 | 6.665 | 18.260 | 1.00 | 59.27 |
| ATOM | 1718 | CZ | ARG | 1661 | 24.952 | 5.369 | 18.471 | 1.00 | 59.83 |
| ATOM | 1719 | NH1 | ARG | 1661 | 24.319 | 4.643 | 17.550 | 1.00 | 57.04 |
| ATOM | 1722 | NH2 | ARG | 1661 | 25.375 | 4.792 | 19.591 | 1.00 | 59.47 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1725 | C | ARG | 1661 | 24.167 | 11.609 | 14.468 | 1.00 | 49.58 |
| ATOM | 1726 | O | ARG | 1661 | 23.169 | 12.321 | 14.375 | 1.00 | 47.38 |
| ATOM | 1727 | N | LEU | 1662 | 24.911 | 11.266 | 13.430 | 1.00 | 46.26 |
| ATOM | 1729 | CA | LEU | 1662 | 24.600 | 11.717 | 12.092 | 1.00 | 44.75 |
| ATOM | 1730 | CB | LEU | 1662 | 25.871 | 12.261 | 11.425 | 1.00 | 43.49 |
| ATOM | 1731 | CG | LEU | 1662 | 26.430 | 13.561 | 12.020 | 1.00 | 43.01 |
| ATOM | 1732 | CD1 | LEU | 1662 | 27.918 | 13.705 | 11.727 | 1.00 | 42.40 |
| ATOM | 1733 | CD2 | LEU | 1662 | 25.644 | 14.760 | 11.507 | 1.00 | 40.19 |
| ATOM | 1734 | C | LEU | 1662 | 23.999 | 10.570 | 11.276 | 1.00 | 43.58 |
| ATOM | 1735 | O | LEU | 1662 | 24.704 | 9.628 | 10.892 | 1.00 | 43.68 |
| ATOM | 1736 | N | PRO | 1663 | 22.680 | 10.631 | 11.010 | 1.00 | 40.72 |
| ATOM | 1737 | CD | PRO | 1663 | 21.723 | 11.629 | 11.521 | 1.00 | 40.27 |
| ATOM | 1738 | CA | PRO | 1663 | 21.981 | 9.603 | 10.237 | 1.00 | 36.86 |
| ATOM | 1739 | CB | PRO | 1663 | 20.595 | 10.214 | 10.035 | 1.00 | 36.67 |
| ATOM | 1740 | CG | PRO | 1663 | 20.375 | 10.937 | 11.314 | 1.00 | 36.84 |
| ATOM | 1741 | C | PRO | 1663 | 22.640 | 9.266 | 8.907 | 1.00 | 33.34 |
| ATOM | 1742 | O | PRO | 1663 | 22.442 | 8.161 | 8.401 | 1.00 | 33.65 |
| ATOM | 1743 | N | VAL | 1664 | 23.427 | 10.188 | 8.343 | 1.00 | 31.26 |
| ATOM | 1745 | CA | VAL | 1664 | 24.095 | 9.915 | 7.058 | 1.00 | 30.43 |
| ATOM | 1746 | CB | VAL | 1664 | 24.887 | 11.125 | 6.466 | 1.00 | 27.09 |
| ATOM | 1747 | CG1 | VAL | 1664 | 23.947 | 12.199 | 6.040 | 1.00 | 23.98 |
| ATOM | 1748 | CG2 | VAL | 1664 | 25.894 | 11.654 | 7.464 | 1.00 | 26.06 |
| ATOM | 1749 | C | VAL | 1664 | 25.044 | 8.728 | 7.163 | 1.00 | 28.18 |
| ATOM | 1750 | O | VAL | 1664 | 25.461 | 8.178 | 6.153 | 1.00 | 28.30 |
| ATOM | 1751 | N | LYS | 1665 | 25.353 | 8.326 | 8.389 | 1.00 | 25.52 |
| ATOM | 1753 | CA | LYS | 1665 | 26.243 | 7.200 | 8.612 | 1.00 | 25.48 |
| ATOM | 1754 | CB | LYS | 1665 | 26.915 | 7.334 | 9.979 | 1.00 | 23.52 |
| ATOM | 1755 | CG | LYS | 1665 | 27.910 | 8.452 | 10.001 | 1.00 | 23.14 |
| ATOM | 1756 | CD | LYS | 1665 | 28.363 | 8.776 | 11.400 | 1.00 | 29.84 |
| ATOM | 1757 | CE | LYS | 1665 | 29.430 | 9.871 | 11.385 | 1.00 | 28.33 |
| ATOM | 1758 | NZ | LYS | 1665 | 29.794 | 10.283 | 12.777 | 1.00 | 30.88 |
| ATOM | 1762 | C | LYS | 1665 | 25.595 | 5.823 | 8.413 | 1.00 | 25.26 |
| ATOM | 1763 | O | LYS | 1665 | 26.261 | 4.798 | 8.512 | 1.00 | 23.05 |
| ATOM | 1764 | N | TRP | 1666 | 24.289 | 5.815 | 8.156 | 1.00 | 27.05 |
| ATOM | 1766 | CA | TRP | 1666 | 23.543 | 4.588 | 7.884 | 1.00 | 27.17 |
| ATOM | 1767 | CB | TRP | 1666 | 22.282 | 4.529 | 8.760 | 1.00 | 26.98 |
| ATOM | 1768 | CG | TRP | 1666 | 22.563 | 4.067 | 10.197 | 1.00 | 29.62 |
| ATOM | 1769 | CD2 | TRP | 1666 | 23.065 | 4.857 | 11.283 | 1.00 | 29.64 |
| ATOM | 1770 | CE2 | TRP | 1666 | 23.230 | 3.988 | 12.393 | 1.00 | 28.25 |
| ATOM | 1771 | CE3 | TRP | 1666 | 23.406 | 6.208 | 11.430 | 1.00 | 29.15 |
| ATOM | 1772 | CD1 | TRP | 1666 | 22.436 | 2.793 | 10.690 | 1.00 | 26.48 |
| ATOM | 1773 | NE1 | TRP | 1666 | 22.834 | 2.737 | 11.997 | 1.00 | 24.81 |
| ATOM | 1775 | CZ2 | TRP | 1666 | 23.719 | 4.430 | 13.636 | 1.00 | 28.40 |
| ATOM | 1776 | CZ3 | TRP | 1666 | 23.894 | 6.647 | 12.670 | 1.00 | 29.38 |
| ATOM | 1777 | CH2 | TRP | 1666 | 24.048 | 5.756 | 13.749 | 1.00 | 29.83 |
| ATOM | 1778 | C | TRP | 1666 | 23.176 | 4.499 | 6.385 | 1.00 | 27.71 |
| ATOM | 1779 | O | TRP | 1666 | 22.745 | 3.451 | 5.900 | 1.00 | 29.42 |
| ATOM | 1780 | N | MET | 1667 | 23.439 | 5.572 | 5.645 | 1.00 | 25.52 |
| ATOM | 1782 | CA | MET | 1667 | 23.098 | 5.642 | 4.232 | 1.00 | 25.24 |
| ATOM | 1783 | CB | MET | 1667 | 22.972 | 7.095 | 3.792 | 1.00 | 26.58 |
| ATOM | 1784 | CG | MET | 1667 | 21.830 | 7.836 | 4.391 | 1.00 | 32.35 |
| ATOM | 1785 | SD | MET | 1667 | 21.846 | 9.559 | 3.877 | 1.00 | 40.32 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1786 | CE | MET | 1667 | 21.033 | 9.447 | 2.341 | 1.00 | 38.17 |
| ATOM | 1787 | C | MET | 1667 | 24.042 | 4.960 | 3.276 | 1.00 | 25.07 |
| ATOM | 1788 | O | MET | 1667 | 25.256 | 5.037 | 3.411 | 1.00 | 27.61 |
| ATOM | 1789 | N | ALA | 1668 | 23.473 | 4.302 | 2.282 | 1.00 | 24.92 |
| ATOM | 1791 | CA | ALA | 1668 | 24.272 | 3.647 | 1.271 | 1.00 | 26.92 |
| ATOM | 1792 | CB | ALA | 1668 | 23.397 | 2.720 | 0.425 | 1.00 | 25.09 |
| ATOM | 1793 | C | ALA | 1668 | 24.866 | 4.759 | 0.410 | 1.00 | 27.82 |
| ATOM | 1794 | O | ALA | 1668 | 24.254 | 5.817 | 0.242 | 1.00 | 27.06 |
| ATOM | 1795 | N | PRO | 1669 | 26.050 | 4.530 | -0.170 | 1.00 | 27.84 |
| ATOM | 1796 | CD | PRO | 1669 | 26.912 | 3.339 | -0.107 | 1.00 | 27.12 |
| ATOM | 1797 | CA | PRO | 1669 | 26.662 | 5.561 | -1.005 | 1.00 | 28.04 |
| ATOM | 1798 | CB | PRO | 1669 | 27.868 | 4.835 | -1.593 | 1.00 | 26.71 |
| ATOM | 1799 | CG | PRO | 1669 | 28.249 | 3.893 | -0.498 | 1.00 | 27.49 |
| ATOM | 1800 | C | PRO | 1669 | 25.734 | 6.078 | -2.108 | 1.00 | 28.51 |
| ATOM | 1801 | O | PRO | 1669 | 25.685 | 7.281 | -2.371 | 1.00 | 30.64 |
| ATOM | 1802 | N | GLU | 1670 | 24.992 | 5.179 | -2.746 | 1.00 | 28.25 |
| ATOM | 1804 | CA | GLU | 1670 | 24.095 | 5.584 | -3.826 | 1.00 | 26.82 |
| ATOM | 1805 | CB | GLU | 1670 | 23.600 | 4.369 | -4.620 | 1.00 | 29.32 |
| ATOM | 1806 | CG | GLU | 1670 | 22.604 | 3.486 | -3.889 | 1.00 | 30.38 |
| ATOM | 1807 | CD | GLU | 1670 | 23.223 | 2.266 | -3.229 | 1.00 | 32.52 |
| ATOM | 1808 | OE1 | GLU | 1670 | 22.444 | 1.393 | -2.794 | 1.00 | 28.06 |
| ATOM | 1809 | OE2 | GLU | 1670 | 24.474 | 2.175 | -3.130 | 1.00 | 28.67 |
| ATOM | 1810 | C | GLU | 1670 | 22.924 | 6.440 | -3.356 | 1.00 | 24.79 |
| ATOM | 1811 | O | GLU | 1670 | 22.410 | 7.236 | -4.123 | 1.00 | 22.31 |
| ATOM | 1812 | N | ALA | 1671 | 22.512 | 6.265 | -2.101 | 1.00 | 26.70 |
| ATOM | 1814 | CA | ALA | 1671 | 21.423 | 7.040 | -1.490 | 1.00 | 25.67 |
| ATOM | 1815 | CB | ALA | 1671 | 20.813 | 6.292 | -0.312 | 1.00 | 18.88 |
| ATOM | 1816 | C | ALA | 1671 | 21.984 | 8.365 | -1.006 | 1.00 | 26.05 |
| ATOM | 1817 | O | ALA | 1671 | 21.400 | 9.414 | -1.229 | 1.00 | 28.14 |
| ATOM | 1818 | N | LEU | 1672 | 23.138 | 8.300 | -0.358 | 1.00 | 29.03 |
| ATOM | 1820 | CA | LEU | 1672 | 23.807 | 9.481 | 0.172 | 1.00 | 34.07 |
| ATOM | 1821 | CB | LEU | 1672 | 25.030 | 9.064 | 0.986 | 1.00 | 34.45 |
| ATOM | 1822 | CG | LEU | 1672 | 25.870 | 10.157 | 1.648 | 1.00 | 39.50 |
| ATOM | 1823 | CD1 | LEU | 1672 | 25.081 | 10.853 | 2.740 | 1.00 | 41.71 |
| ATOM | 1824 | CD2 | LEU | 1672 | 27.123 | 9.530 | 2.243 | 1.00 | 40.16 |
| ATOM | 1825 | C | LEU | 1672 | 24.248 | 10.431 | -0.942 | 1.00 | 38.47 |
| ATOM | 1826 | O | LEU | 1672 | 23.958 | 11.625 | -0.898 | 1.00 | 42.25 |
| ATOM | 1827 | N | PHE | 1673 | 24.924 | 9.901 | -1.956 | 1.00 | 39.07 |
| ATOM | 1829 | CA | PHE | 1673 | 25.414 | 10.725 | -3.053 | 1.00 | 38.00 |
| ATOM | 1830 | CB | PHE | 1673 | 26.699 | 10.110 | -3.639 | 1.00 | 36.48 |
| ATOM | 1831 | CG | PHE | 1673 | 27.826 | 9.928 | -2.637 | 1.00 | 33.36 |
| ATOM | 1832 | CD1 | PHE | 1673 | 28.524 | 8.724 | -2.580 | 1.00 | 29.55 |
| ATOM | 1833 | CD2 | PHE | 1673 | 28.205 | 10.960 | -1.779 | 1.00 | 31.85 |
| ATOM | 1834 | CE1 | PHE | 1673 | 29.580 | 8.540 | -1.692 | 1.00 | 26.33 |
| ATOM | 1835 | CE2 | PHE | 1673 | 29.265 | 10.786 | -0.880 | 1.00 | 30.95 |
| ATOM | 1836 | CZ | PHE | 1673 | 29.954 | 9.568 | -0.838 | 1.00 | 28.99 |
| ATOM | 1837 | C | PHE | 1673 | 24.413 | 10.957 | -4.194 | 1.00 | 39.64 |
| ATOM | 1838 | O | PHE | 1673 | 24.364 | 12.046 | -4.760 | 1.00 | 37.72 |
| ATOM | 1839 | N | ASP | 1674 | 23.651 | 9.928 | -4.554 | 1.00 | 41.35 |
| ATOM | 1841 | CA | ASP | 1674 | 22.716 | 10.027 | -5.666 | 1.00 | 43.38 |
| ATOM | 1842 | CB | ASP | 1674 | 22.934 | 8.858 | -6.625 | 1.00 | 47.84 |
| ATOM | 1843 | CG | ASP | 1674 | 24.359 | 8.765 | -7.121 | 1.00 | 53.24 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1844 | OD1 | ASP | 1674 | 25.049 | 9.808 | -7.172 | 1.00 | 56.20 |
| ATOM | 1845 | OD2 | ASP | 1674 | 24.786 | 7.640 | -7.460 | 1.00 | 55.73 |
| ATOM | 1846 | C | ASP | 1674 | 21.239 | 10.083 | -5.321 | 1.00 | 45.94 |
| ATOM | 1847 | O | ASP | 1674 | 20.402 | 10.200 | -6.222 | 1.00 | 47.80 |
| ATOM | 1848 | N | ARG | 1675 | 20.903 | 9.953 | -4.040 | 1.00 | 45.98 |
| ATOM | 1850 | CA | ARG | 1675 | 19.503 | 9.981 | -3.608 | 1.00 | 43.76 |
| ATOM | 1851 | CB | ARG | 1675 | 18.872 | 11.346 | -3.887 | 1.00 | 48.61 |
| ATOM | 1852 | CG | ARG | 1675 | 19.519 | 12.478 | -3.142 | 1.00 | 58.37 |
| ATOM | 1853 | CD | ARG | 1675 | 19.468 | 13.715 | -3.992 | 1.00 | 70.39 |
| ATOM | 1854 | NE | ARG | 1675 | 20.035 | 14.867 | -3.306 | 1.00 | 79.14 |
| ATOM | 1856 | CZ | ARG | 1675 | 19.612 | 16.116 | -3.472 | 1.00 | 82.95 |
| ATOM | 1857 | NH1 | ARG | 1675 | 18.610 | 16.386 | -4.308 | 1.00 | 82.00 |
| ATOM | 1860 | NH2 | ARG | 1675 | 20.194 | 17.097 | -2.793 | 1.00 | 87.42 |
| ATOM | 1863 | C | ARG | 1675 | 18.647 | 8.882 | -4.236 | 1.00 | 39.26 |
| ATOM | 1864 | O | ARG | 1675 | 17.461 | 9.074 | -4.488 | 1.00 | 37.29 |
| ATOM | 1865 | N | ILE | 1676 | 19.270 | 7.746 | -4.526 | 1.00 | 35.86 |
| ATOM | 1867 | CA | ILE | 1676 | 18.544 | 6.614 | -5.081 | 1.00 | 32.76 |
| ATOM | 1868 | CB | ILE | 1676 | 19.324 | 5.927 | -6.192 | 1.00 | 31.73 |
| ATOM | 1869 | CG2 | ILE | 1676 | 18.450 | 4.902 | -6.868 | 1.00 | 30.02 |
| ATOM | 1870 | CG1 | ILE | 1676 | 19.767 | 6.955 | -7.219 | 1.00 | 32.68 |
| ATOM | 1871 | CD1 | ILE | 1676 | 20.658 | 6.371 | -8.272 | 1.00 | 35.75 |
| ATOM | 1872 | C | ILE | 1676 | 18.329 | 5.625 | -3.946 | 1.00 | 31.08 |
| ATOM | 1873 | O | ILE | 1676 | 19.264 | 4.962 | -3.505 | 1.00 | 28.77 |
| ATOM | 1874 | N | TYR | 1677 | 17.102 | 5.558 | -3.444 | 1.00 | 30.32 |
| ATOM | 1876 | CA | TYR | 1677 | 16.779 | 4.653 | -2.348 | 1.00 | 29.68 |
| ATOM | 1877 | CB | TYR | 1677 | 15.846 | 5.329 | -1.354 | 1.00 | 31.14 |
| ATOM | 1878 | CG | TYR | 1677 | 16.523 | 6.395 | -0.514 | 1.00 | 32.95 |
| ATOM | 1879 | CD1 | TYR | 1677 | 16.616 | 7.721 | -0.958 | 1.00 | 30.40 |
| ATOM | 1880 | CE1 | TYR | 1677 | 17.208 | 8.707 | -0.171 | 1.00 | 27.57 |
| ATOM | 1881 | CD2 | TYR | 1677 | 17.048 | 6.082 | 0.743 | 1.00 | 32.13 |
| ATOM | 1882 | CE2 | TYR | 1677 | 17.642 | 7.059 | 1.543 | 1.00 | 31.50 |
| ATOM | 1883 | CZ | TYR | 1677 | 17.711 | 8.366 | 1.081 | 1.00 | 31.12 |
| ATOM | 1884 | OH | TYR | 1677 | 18.235 | 9.326 | 1.912 | 1.00 | 32.18 |
| ATOM | 1886 | C | TYR | 1677 | 16.123 | 3.424 | -2.933 | 1.00 | 28.88 |
| ATOM | 1887 | O | TYR | 1677 | 15.268 | 3.537 | -3.811 | 1.00 | 32.20 |
| ATOM | 1888 | N | THR | 1678 | 16.556 | 2.253 | -2.481 | 1.00 | 26.34 |
| ATOM | 1890 | CA | THR | 1678 | 16.023 | 0.988 | -2.971 | 1.00 | 25.55 |
| ATOM | 1891 | CB | THR | 1678 | 16.917 | 0.394 | -4.043 | 1.00 | 28.81 |
| ATOM | 1892 | OG1 | THR | 1678 | 18.221 | 0.179 | -3.483 | 1.00 | 34.06 |
| ATOM | 1894 | CG2 | THR | 1678 | 17.010 | 1.320 | -5.267 | 1.00 | 27.25 |
| ATOM | 1895 | C | THR | 1678 | 16.037 | 0.007 | -1.827 | 1.00 | 21.78 |
| ATOM | 1896 | O | THR | 1678 | 16.505 | 0.312 | -0.744 | 1.00 | 25.57 |
| ATOM | 1897 | N | HIS | 1679 | 15.559 | -1.198 | -2.071 | 1.00 | 20.86 |
| ATOM | 1899 | CA | HIS | 1679 | 15.580 | -2.216 | -1.030 | 1.00 | 20.30 |
| ATOM | 1900 | CB | HIS | 1679 | 14.816 | -3.453 | -1.499 | 1.00 | 17.22 |
| ATOM | 1901 | CG | HIS | 1679 | 13.367 | -3.196 | -1.797 | 1.00 | 19.02 |
| ATOM | 1902 | CD2 | HIS | 1679 | 12.662 | -3.275 | -2.958 | 1.00 | 14.89 |
| ATOM | 1903 | ND1 | HIS | 1679 | 12.459 | -2.830 | -0.826 | 1.00 | 18.98 |
| ATOM | 1905 | CE1 | HIS | 1679 | 11.260 | -2.697 | -1.370 | 1.00 | 16.10 |
| ATOM | 1906 | NE2 | HIS | 1679 | 11.359 | -2.961 | -2.663 | 1.00 | 15.18 |
| ATOM | 1908 | C | HIS | 1679 | 17.050 | -2.535 | -0.761 | 1.00 | 20.44 |
| ATOM | 1909 | O | HIS | 1679 | 17.428 | -2.901 | 0.356 | 1.00 | 22.58 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1910 | N | GLN | 1680 | 17.874 | -2.310 | -1.781 | 1.00 | 20.58 |
| ATOM | 1912 | CA | GLN | 1680 | 19.303 | -2.539 | -1.721 | 1.00 | 22.70 |
| ATOM | 1913 | CB | GLN | 1680 | 19.935 | -2.427 | -3.106 | 1.00 | 26.26 |
| ATOM | 1914 | CG | GLN | 1680 | 19.934 | -3.711 | -3.889 | 1.00 | 31.86 |
| ATOM | 1915 | CD | GLN | 1680 | 18.949 | -3.687 | -5.026 | 1.00 | 37.54 |
| ATOM | 1916 | OE1 | GLN | 1680 | 17.931 | -3.000 | -4.961 | 1.00 | 42.70 |
| ATOM | 1917 | NE2 | GLN | 1680 | 19.256 | -4.409 | -6.091 | 1.00 | 37.42 |
| ATOM | 1920 | C | GLN | 1680 | 19.985 | -1.559 | -0.797 | 1.00 | 24.93 |
| ATOM | 1921 | O | GLN | 1680 | 20.875 | -1.943 | -0.039 | 1.00 | 26.39 |
| ATOM | 1922 | N | SER | 1681 | 19.605 | -0.286 | -0.867 | 1.00 | 24.70 |
| ATOM | 1924 | CA | SER | 1681 | 20.239 | 0.678 | 0.030 | 1.00 | 23.24 |
| ATOM | 1925 | CB | SER | 1681 | 19.923 | 2.128 | -0.346 | 1.00 | 19.33 |
| ATOM | 1926 | OG | SER | 1681 | 18.544 | 2.326 | -0.545 | 1.00 | 18.55 |
| ATOM | 1928 | C | SER | 1681 | 19.852 | 0.364 | 1.464 | 1.00 | 21.77 |
| ATOM | 1929 | O | SER | 1681 | 20.645 | 0.609 | 2.366 | 1.00 | 24.14 |
| ATOM | 1930 | N | ASP | 1682 | 18.659 | -0.210 | 1.670 | 1.00 | 21.80 |
| ATOM | 1932 | CA | ASP | 1682 | 18.180 | -0.604 | 3.003 | 1.00 | 22.45 |
| ATOM | 1933 | CB | ASP | 1682 | 16.730 | -1.111 | 2.963 | 1.00 | 25.27 |
| ATOM | 1934 | CG | ASP | 1682 | 15.678 | 0.004 | 3.132 | 1.00 | 28.21 |
| ATOM | 1935 | OD1 | ASP | 1682 | 14.500 | -0.245 | 2.786 | 1.00 | 25.41 |
| ATOM | 1936 | OD2 | ASP | 1682 | 15.992 | 1.102 | 3.639 | 1.00 | 30.19 |
| ATOM | 1937 | C | ASP | 1682 | 19.076 | -1.736 | 3.517 | 1.00 | 23.69 |
| ATOM | 1938 | O | ASP | 1682 | 19.385 | -1.799 | 4.709 | 1.00 | 24.74 |
| ATOM | 1939 | N | VAL | 1683 | 19.474 | -2.635 | 2.620 | 1.00 | 23.49 |
| ATOM | 1941 | CA | VAL | 1683 | 20.354 | -3.737 | 3.003 | 1.00 | 21.77 |
| ATOM | 1942 | CB | VAL | 1683 | 20.543 | -4.741 | 1.837 | 1.00 | 20.49 |
| ATOM | 1943 | CG1 | VAL | 1683 | 21.770 | -5.613 | 2.039 | 1.00 | 19.82 |
| ATOM | 1944 | CG2 | VAL | 1683 | 19.320 | -5.618 | 1.736 | 1.00 | 19.29 |
| ATOM | 1945 | C | VAL | 1683 | 21.674 | -3.153 | 3.523 | 1.00 | 21.93 |
| ATOM | 1946 | O | VAL | 1683 | 22.161 | -3.570 | 4.573 | 1.00 | 21.06 |
| ATOM | 1947 | N | TRP | 1684 | 22.207 | -2.143 | 2.837 | 1.00 | 20.64 |
| ATOM | 1949 | CA | TRP | 1684 | 23.424 | -1.482 | 3.295 | 1.00 | 20.98 |
| ATOM | 1950 | CB | TRP | 1684 | 23.711 | -0.224 | 2.463 | 1.00 | 19.56 |
| ATOM | 1951 | CG | TRP | 1684 | 24.859 | 0.609 | 2.970 | 1.00 | 23.22 |
| ATOM | 1952 | CD2 | TRP | 1684 | 26.182 | 0.686 | 2.421 | 1.00 | 24.64 |
| ATOM | 1953 | CE2 | TRP | 1684 | 26.929 | 1.559 | 3.249 | 1.00 | 24.69 |
| ATOM | 1954 | CE3 | TRP | 1684 | 26.813 | 0.102 | 1.315 | 1.00 | 26.41 |
| ATOM | 1955 | CD1 | TRP | 1684 | 24.857 | 1.430 | 4.075 | 1.00 | 23.64 |
| ATOM | 1956 | NE1 | TRP | 1684 | 26.097 | 1.994 | 4.246 | 1.00 | 23.28 |
| ATOM | 1958 | CZ2 | TRP | 1684 | 28.275 | 1.859 | 3.000 | 1.00 | 20.55 |
| ATOM | 1959 | CZ3 | TRP | 1684 | 28.165 | 0.409 | 1.072 | 1.00 | 22.82 |
| ATOM | 1960 | CH2 | TRP | 1684 | 28.872 | 1.274 | 1.908 | 1.00 | 19.24 |
| ATOM | 1961 | C | TRP | 1684 | 23.201 | -1.112 | 4.771 | 1.00 | 21.12 |
| ATOM | 1962 | O | TRP | 1684 | 23.931 | -1.560 | 5.652 | 1.00 | 22.08 |
| ATOM | 1963 | N | SER | 1685 | 22.150 | -0.342 | 5.032 | 1.00 | 23.27 |
| ATOM | 1965 | CA | SER | 1685 | 21.787 | 0.086 | 6.386 | 1.00 | 22.54 |
| ATOM | 1966 | CB | SER | 1685 | 20.429 | 0.768 | 6.356 | 1.00 | 21.98 |
| ATOM | 1967 | OG | SER | 1685 | 20.318 | 1.626 | 5.220 | 1.00 | 25.48 |
| ATOM | 1969 | C | SER | 1685 | 21.747 | -1.068 | 7.389 | 1.00 | 21.33 |
| ATOM | 1970 | O | SER | 1685 | 22.145 | -0.902 | 8.545 | 1.00 | 19.52 |
| ATOM | 1971 | N | PHE | 1686 | 21.260 | -2.228 | 6.946 | 1.00 | 23.10 |
| ATOM | 1973 | CA | PHE | 1686 | 21.174 | -3.424 | 7.800 | 1.00 | 23.09 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1974 | CB | PHE | 1686 | 20.409 | -4.550 | 7.095 | 1.00 | 22.77 |
| ATOM | 1975 | CG | PHE | 1686 | 20.192 | -5.767 | 7.962 | 1.00 | 25.82 |
| ATOM | 1976 | CD1 | PHE | 1686 | 19.378 | -5.694 | 9.096 | 1.00 | 25.54 |
| ATOM | 1977 | CD2 | PHE | 1686 | 20.808 | -6.987 | 7.649 | 1.00 | 23.88 |
| ATOM | 1978 | CE1 | PHE | 1686 | 19.185 | -6.809 | 9.913 | 1.00 | 24.25 |
| ATOM | 1979 | CE2 | PHE | 1686 | 20.622 | -8.109 | 8.455 | 1.00 | 22.67 |
| ATOM | 1980 | CZ | PHE | 1686 | 19.809 | -8.023 | 9.585 | 1.00 | 26.30 |
| ATOM | 1981 | C | PHE | 1686 | 22.569 | -3.919 | 8.240 | 1.00 | 21.77 |
| ATOM | 1982 | O | PHE | 1686 | 22.739 | -4.450 | 9.350 | 1.00 | 20.47 |
| ATOM | 1983 | N | GLY | 1687 | 23.553 | -3.773 | 7.358 | 1.00 | 20.63 |
| ATOM | 1985 | CA | GLY | 1687 | 24.913 | -4.163 | 7.685 | 1.00 | 19.29 |
| ATOM | 1986 | C | GLY | 1687 | 25.407 | -3.276 | 8.822 | 1.00 | 21.64 |
| ATOM | 1987 | O | GLY | 1687 | 26.094 | -3.755 | 9.727 | 1.00 | 19.46 |
| ATOM | 1988 | N | VAL | 1688 | 25.008 | -1.996 | 8.794 | 1.00 | 22.19 |
| ATOM | 1990 | CA | VAL | 1688 | 25.372 | -1.024 | 9.831 | 1.00 | 21.99 |
| ATOM | 1991 | CB | VAL | 1688 | 25.048 | 0.458 | 9.423 | 1.00 | 23.20 |
| ATOM | 1992 | CG1 | VAL | 1688 | 25.439 | 1.424 | 10.540 | 1.00 | 21.22 |
| ATOM | 1993 | CG2 | VAL | 1688 | 25.820 | 0.846 | 8.161 | 1.00 | 21.25 |
| ATOM | 1994 | C | VAL | 1688 | 24.621 | -1.403 | 11.100 | 1.00 | 23.33 |
| ATOM | 1995 | O | VAL | 1688 | 25.204 | -1.420 | 12.187 | 1.00 | 24.98 |
| ATOM | 1996 | N | LEU | 1689 | 23.339 | -1.734 | 10.969 | 1.00 | 24.36 |
| ATOM | 1998 | CA | LEU | 1689 | 22.542 | -2.161 | 12.122 | 1.00 | 23.92 |
| ATOM | 1999 | CB | LEU | 1689 | 21.072 | -2.392 | 11.714 | 1.00 | 22.57 |
| ATOM | 2000 | CG | LEU | 1689 | 19.981 | -2.427 | 12.805 | 1.00 | 23.41 |
| ATOM | 2001 | CD1 | LEU | 1689 | 18.614 | -2.295 | 12.164 | 1.00 | 19.14 |
| ATOM | 2002 | CD2 | LEU | 1689 | 20.048 | -3.700 | 13.658 | 1.00 | 22.75 |
| ATOM | 2003 | C | LEU | 1689 | 23.158 | -3.447 | 12.717 | 1.00 | 25.22 |
| ATOM | 2004 | O | LEU | 1689 | 23.202 | -3.592 | 13.937 | 1.00 | 25.58 |
| ATOM | 2005 | N | LEU | 1690 | 23.614 | -4.379 | 11.871 | 1.00 | 25.47 |
| ATOM | 2007 | CA | LEU | 1690 | 24.256 | -5.604 | 12.376 | 1.00 | 26.26 |
| ATOM | 2008 | CB | LEU | 1690 | 24.730 | -6.531 | 11.255 | 1.00 | 26.22 |
| ATOM | 2009 | CG | LEU | 1690 | 23.809 | -7.501 | 10.515 | 1.00 | 26.21 |
| ATOM | 2010 | CD1 | LEU | 1690 | 24.662 | -8.259 | 9.523 | 1.00 | 25.45 |
| ATOM | 2011 | CD2 | LEU | 1690 | 23.135 | -8.487 | 11.458 | 1.00 | 21.17 |
| ATOM | 2012 | C | LEU | 1690 | 25.471 | -5.204 | 13.189 | 1.00 | 26.51 |
| ATOM | 2013 | O | LEU | 1690 | 25.710 | -5.747 | 14.273 | 1.00 | 29.07 |
| ATOM | 2014 | N | TRP | 1691 | 26.240 | -4.255 | 12.660 | 1.00 | 26.26 |
| ATOM | 2016 | CA | TRP | 1691 | 27.431 | -3.761 | 13.341 | 1.00 | 25.08 |
| ATOM | 2017 | CB | TRP | 1691 | 28.129 | -2.706 | 12.493 | 1.00 | 25.16 |
| ATOM | 2018 | CG | TRP | 1691 | 29.456 | -2.268 | 13.039 | 1.00 | 27.49 |
| ATOM | 2019 | CD2 | TRP | 1691 | 29.701 | -1.163 | 13.925 | 1.00 | 25.81 |
| ATOM | 2020 | CE2 | TRP | 1691 | 31.100 | -1.070 | 14.103 | 1.00 | 22.63 |
| ATOM | 2021 | CE3 | TRP | 1691 | 28.870 | -0.236 | 14.575 | 1.00 | 26.70 |
| ATOM | 2022 | CD1 | TRP | 1691 | 30.688 | -2.798 | 12.735 | 1.00 | 23.03 |
| ATOM | 2023 | NE1 | TRP | 1691 | 31.675 | -2.078 | 13.371 | 1.00 | 25.19 |
| ATOM | 2025 | CZ2 | TRP | 1691 | 31.690 | -0.085 | 14.900 | 1.00 | 18.66 |
| ATOM | 2026 | CZ3 | TRP | 1691 | 29.459 | 0.745 | 15.371 | 1.00 | 25.66 |
| ATOM | 2027 | CH2 | TRP | 1691 | 30.861 | 0.812 | 15.523 | 1.00 | 23.00 |
| ATOM | 2028 | C | TRP | 1691 | 27.114 | -3.195 | 14.727 | 1.00 | 24.63 |
| ATOM | 2029 | O | TRP | 1691 | 27.871 | -3.393 | 15.662 | 1.00 | 27.79 |
| ATOM | 2030 | N | GLU | 1692 | 25.985 | -2.506 | 14.862 | 1.00 | 26.48 |
| ATOM | 2032 | CA | GLU | 1692 | 25.574 | -1.938 | 16.155 | 1.00 | 24.98 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2033 | CB | GLU | 1692 | 24.335 | -1.060 | 15.994 | 1.00 | 22.29 |
| ATOM | 2034 | CG | GLU | 1692 | 24.507 | 0.107 | 15.056 | 1.00 | 18.31 |
| ATOM | 2035 | CD | GLU | 1692 | 23.255 | 0.933 | 14.978 | 1.00 | 25.10 |
| ATOM | 2036 | OE1 | GLU | 1692 | 22.433 | 0.704 | 14.066 | 1.00 | 26.95 |
| ATOM | 2037 | OE2 | GLU | 1692 | 23.067 | 1.815 | 15.840 | 1.00 | 27.05 |
| ATOM | 2038 | C | GLU | 1692 | 25.260 | -3.036 | 17.163 | 1.00 | 25.18 |
| ATOM | 2039 | O | GLU | 1692 | 25.602 | -2.927 | 18.341 | 1.00 | 26.12 |
| ATOM | 2040 | N | ILE | 1693 | 24.593 | -4.087 | 16.698 | 1.00 | 27.16 |
| ATOM | 2042 | CA | ILE | 1693 | 24.231 | -5.214 | 17.555 | 1.00 | 25.91 |
| ATOM | 2043 | CB | ILE | 1693 | 23.373 | -6.287 | 16.777 | 1.00 | 25.70 |
| ATOM | 2044 | CG2 | ILE | 1693 | 23.171 | -7.564 | 17.638 | 1.00 | 18.73 |
| ATOM | 2045 | CG1 | ILE | 1693 | 22.005 | -5.682 | 16.382 | 1.00 | 23.45 |
| ATOM | 2046 | CD1 | ILE | 1693 | 21.208 | -6.485 | 15.346 | 1.00 | 15.62 |
| ATOM | 2047 | C | ILE | 1693 | 25.496 | -5.847 | 18.107 | 1.00 | 26.70 |
| ATOM | 2048 | O | ILE | 1693 | 25.672 | -5.961 | 19.316 | 1.00 | 28.19 |
| ATOM | 2049 | N | PHE | 1694 | 26.442 | -6.133 | 17.229 | 1.00 | 28.78 |
| ATOM | 2051 | CA | PHE | 1694 | 27.664 | -6.779 | 17.679 | 1.00 | 29.72 |
| ATOM | 2052 | CB | PHE | 1694 | 28.261 | -7.598 | 16.542 | 1.00 | 27.18 |
| ATOM | 2053 | CG | PHE | 1694 | 27.315 | -8.649 | 16.048 | 1.00 | 25.38 |
| ATOM | 2054 | CD1 | PHE | 1694 | 26.793 | -8.599 | 14.770 | 1.00 | 26.16 |
| ATOM | 2055 | CD2 | PHE | 1694 | 26.844 | -9.625 | 16.919 | 1.00 | 26.37 |
| ATOM | 2056 | CE1 | PHE | 1694 | 25.808 | -9.505 | 14.370 | 1.00 | 31.37 |
| ATOM | 2057 | CE2 | PHE | 1694 | 25.863 | -10.533 | 16.536 | 1.00 | 25.23 |
| ATOM | 2058 | CZ | PHE | 1694 | 25.337 | -10.478 | 15.268 | 1.00 | 29.46 |
| ATOM | 2059 | C | PHE | 1694 | 28.663 | -5.906 | 18.438 | 1.00 | 30.92 |
| ATOM | 2060 | O | PHE | 1694 | 29.697 | -6.403 | 18.902 | 1.00 | 32.23 |
| ATOM | 2061 | N | THR | 1695 | 28.344 | -4.616 | 18.575 | 1.00 | 29.46 |
| ATOM | 2063 | CA | THR | 1695 | 29.170 | -3.698 | 19.348 | 1.00 | 27.17 |
| ATOM | 2064 | CB | THR | 1695 | 29.665 | -2.474 | 18.535 | 1.00 | 23.32 |
| ATOM | 2065 | OG1 | THR | 1695 | 28.553 | -1.710 | 18.046 | 1.00 | 24.73 |
| ATOM | 2067 | CG2 | THR | 1695 | 30.538 | -2.914 | 17.395 | 1.00 | 21.34 |
| ATOM | 2068 | C | THR | 1695 | 28.307 | -3.230 | 20.519 | 1.00 | 28.81 |
| ATOM | 2069 | O | THR | 1695 | 28.707 | -2.346 | 21.289 | 1.00 | 31.85 |
| ATOM | 2070 | N | LEU | 1696 | 27.130 | -3.841 | 20.651 | 1.00 | 26.30 |
| ATOM | 2072 | CA | LEU | 1696 | 26.188 | -3.523 | 21.720 | 1.00 | 25.99 |
| ATOM | 2073 | CB | LEU | 1696 | 26.704 | -4.043 | 23.060 | 1.00 | 24.51 |
| ATOM | 2074 | CG | LEU | 1696 | 26.974 | -5.539 | 23.194 | 1.00 | 23.32 |
| ATOM | 2075 | CD1 | LEU | 1696 | 27.447 | -5.843 | 24.597 | 1.00 | 26.45 |
| ATOM | 2076 | CD2 | LEU | 1696 | 25.726 | -6.297 | 22.907 | 1.00 | 29.79 |
| ATOM | 2077 | C | LEU | 1696 | 25.892 | -2.036 | 21.837 | 1.00 | 24.90 |
| ATOM | 2078 | O | LEU | 1696 | 26.083 | -1.457 | 22.889 | 1.00 | 28.99 |
| ATOM | 2079 | N | GLY | 1697 | 25.386 | -1.432 | 20.771 | 1.00 | 25.05 |
| ATOM | 2081 | CA | GLY | 1697 | 25.072 | -0.016 | 20.811 | 1.00 | 24.31 |
| ATOM | 2082 | C | GLY | 1697 | 26.241 | 0.847 | 20.381 | 1.00 | 27.15 |
| ATOM | 2083 | O | GLY | 1697 | 26.297 | 2.035 | 20.701 | 1.00 | 29.57 |
| ATOM | 2084 | N | GLY | 1698 | 27.177 | 0.261 | 19.639 | 1.00 | 27.33 |
| ATOM | 2086 | CA | GLY | 1698 | 28.319 | 1.023 | 19.178 | 1.00 | 27.04 |
| ATOM | 2087 | C | GLY | 1698 | 27.966 | 2.109 | 18.173 | 1.00 | 29.78 |
| ATOM | 2088 | O | GLY | 1698 | 27.115 | 1.929 | 17.301 | 1.00 | 32.03 |
| ATOM | 2089 | N | SER | 1699 | 28.633 | 3.247 | 18.295 | 1.00 | 30.60 |
| ATOM | 2091 | CA | SER | 1699 | 28.413 | 4.385 | 17.414 | 1.00 | 31.48 |
| ATOM | 2092 | CB | SER | 1699 | 28.747 | 5.692 | 18.164 | 1.00 | 32.97 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2093 | OG | SER | 1699 | 28.350 | 6.848 | 17.436 | 1.00 | 37.75 |
| ATOM | 2095 | C | SER | 1699 | 29.323 | 4.239 | 16.188 | 1.00 | 32.74 |
| ATOM | 2096 | O | SER | 1699 | 30.541 | 4.034 | 16.321 | 1.00 | 33.04 |
| ATOM | 2097 | N | PRO | 1700 | 28.732 | 4.276 | 14.979 | 1.00 | 31.40 |
| ATOM | 2098 | CD | PRO | 1700 | 27.288 | 4.320 | 14.688 | 1.00 | 30.88 |
| ATOM | 2099 | CA | PRO | 1700 | 29.507 | 4.153 | 13.737 | 1.00 | 30.55 |
| ATOM | 2100 | CB | PRO | 1700 | 28.420 | 4.024 | 12.657 | 1.00 | 30.13 |
| ATOM | 2101 | CG | PRO | 1700 | 27.228 | 3.535 | 13.398 | 1.00 | 31.10 |
| ATOM | 2102 | C | PRO | 1700 | 30.300 | 5.427 | 13.509 | 1.00 | 31.19 |
| ATOM | 2103 | O | PRO | 1700 | 29.766 | 6.522 | 13.651 | 1.00 | 35.48 |
| ATOM | 2104 | N | TYR | 1701 | 31.574 | 5.277 | 13.175 | 1.00 | 29.51 |
| ATOM | 2106 | CA | TYR | 1701 | 32.446 | 6.412 | 12.899 | 1.00 | 30.10 |
| ATOM | 2107 | CB | TYR | 1701 | 32.084 | 7.029 | 11.541 | 1.00 | 32.84 |
| ATOM | 2108 | CG | TYR | 1701 | 32.102 | 6.078 | 10.353 | 1.00 | 38.43 |
| ATOM | 2109 | CD1 | TYR | 1701 | 30.921 | 5.795 | 9.643 | 1.00 | 40.14 |
| ATOM | 2110 | CE1 | TYR | 1701 | 30.930 | 5.000 | 8.513 | 1.00 | 39.07 |
| ATOM | 2111 | CD2 | TYR | 1701 | 33.298 | 5.522 | 9.890 | 1.00 | 38.19 |
| ATOM | 2112 | CE2 | TYR | 1701 | 33.320 | 4.726 | 8.754 | 1.00 | 41.52 |
| ATOM | 2113 | CZ | TYR | 1701 | 32.134 | 4.471 | 8.067 | 1.00 | 44.97 |
| ATOM | 2114 | OH | TYR | 1701 | 32.151 | 3.700 | 6.919 | 1.00 | 54.77 |
| ATOM | 2116 | C | TYR | 1701 | 32.426 | 7.524 | 13.965 | 1.00 | 30.38 |
| ATOM | 2117 | O | TYR | 1701 | 32.009 | 8.655 | 13.685 | 1.00 | 30.54 |
| ATOM | 2118 | N | PRO | 1702 | 32.947 | 7.239 | 15.170 | 1.00 | 30.61 |
| ATOM | 2119 | CD | PRO | 1702 | 33.578 | 5.985 | 15.608 | 1.00 | 29.72 |
| ATOM | 2120 | CA | PRO | 1702 | 32.971 | 8.239 | 16.248 | 1.00 | 28.48 |
| ATOM | 2121 | CB | PRO | 1702 | 33.554 | 7.463 | 17.429 | 1.00 | 28.43 |
| ATOM | 2122 | CG | PRO | 1702 | 33.320 | 6.025 | 17.085 | 1.00 | 30.63 |
| ATOM | 2123 | C | PRO | 1702 | 33.897 | 9.385 | 15.881 | 1.00 | 26.93 |
| ATOM | 2124 | O | PRO | 1702 | 34.998 | 9.156 | 15.418 | 1.00 | 26.21 |
| ATOM | 2125 | N | GLY | 1703 | 33.440 | 10.613 | 16.084 | 1.00 | 29.51 |
| ATOM | 2127 | CA | GLY | 1703 | 34.239 | 11.787 | 15.767 | 1.00 | 28.57 |
| ATOM | 2128 | C | GLY | 1703 | 34.374 | 12.143 | 14.296 | 1.00 | 28.97 |
| ATOM | 2129 | O | GLY | 1703 | 35.055 | 13.104 | 13.962 | 1.00 | 29.54 |
| ATOM | 2130 | N | VAL | 1704 | 33.726 | 11.380 | 13.418 | 1.00 | 30.90 |
| ATOM | 2132 | CA | VAL | 1704 | 33.798 | 11.616 | 11.975 | 1.00 | 29.48 |
| ATOM | 2133 | CB | VAL | 1704 | 33.806 | 10.289 | 11.228 | 1.00 | 28.23 |
| ATOM | 2134 | CG1 | VAL | 1704 | 34.074 | 10.525 | 9.750 | 1.00 | 31.57 |
| ATOM | 2135 | CG2 | VAL | 1704 | 34.851 | 9.375 | 11.822 | 1.00 | 28.40 |
| ATOM | 2136 | C | VAL | 1704 | 32.620 | 12.466 | 11.477 | 1.00 | 33.14 |
| ATOM | 2137 | O | VAL | 1704 | 31.466 | 12.045 | 11.529 | 1.00 | 35.67 |
| ATOM | 2138 | N | PRO | 1705 | 32.906 | 13.681 | 10.979 | 1.00 | 35.22 |
| ATOM | 2139 | CD | PRO | 1705 | 34.217 | 14.348 | 11.008 | 1.00 | 38.03 |
| ATOM | 2140 | CA | PRO | 1705 | 31.868 | 14.587 | 10.474 | 1.00 | 35.96 |
| ATOM | 2141 | CB | PRO | 1705 | 32.534 | 15.953 | 10.627 | 1.00 | 35.84 |
| ATOM | 2142 | CG | PRO | 1705 | 33.939 | 15.661 | 10.279 | 1.00 | 37.29 |
| ATOM | 2143 | C | PRO | 1705 | 31.473 | 14.293 | 9.031 | 1.00 | 37.17 |
| ATOM | 2144 | O | PRO | 1705 | 32.255 | 13.690 | 8.288 | 1.00 | 38.39 |
| ATOM | 2145 | N | VAL | 1706 | 30.296 | 14.780 | 8.624 | 1.00 | 36.10 |
| ATOM | 2147 | CA | VAL | 1706 | 29.743 | 14.582 | 7.276 | 1.00 | 37.10 |
| ATOM | 2148 | CB | VAL | 1706 | 28.667 | 15.658 | 6.942 | 1.00 | 38.36 |
| ATOM | 2149 | CG1 | VAL | 1706 | 28.106 | 15.441 | 5.535 | 1.00 | 38.93 |
| ATOM | 2150 | CG2 | VAL | 1706 | 27.536 | 15.595 | 7.952 | 1.00 | 40.79 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2151 | C | VAL | 1706 | 30.762 | 14.559 | 6.138 | 1.00 | 37.09 |
| ATOM | 2152 | O | VAL | 1706 | 30.927 | 13.543 | 5.461 | 1.00 | 38.75 |
| ATOM | 2153 | N | GLU | 1707 | 31.477 | 15.663 | 5.967 | 1.00 | 37.08 |
| ATOM | 2155 | CA | GLU | 1707 | 32.472 | 15.793 | 4.910 | 1.00 | 35.52 |
| ATOM | 2156 | CB | GLU | 1707 | 33.059 | 17.206 | 4.918 | 1.00 | 38.30 |
| ATOM | 2157 | C | GLU | 1707 | 33.588 | 14.762 | 4.945 | 1.00 | 34.20 |
| ATOM | 2158 | O | GLU | 1707 | 34.153 | 14.445 | 3.908 | 1.00 | 33.48 |
| ATOM | 2159 | N | GLU | 1708 | 33.936 | 14.273 | 6.132 | 1.00 | 34.20 |
| ATOM | 2161 | CA | GLU | 1708 | 34.981 | 13.256 | 6.241 | 1.00 | 36.08 |
| ATOM | 2162 | CB | GLU | 1708 | 35.555 | 13.178 | 7.660 | 1.00 | 40.39 |
| ATOM | 2163 | CG | GLU | 1708 | 36.212 | 14.464 | 8.179 | 1.00 | 45.41 |
| ATOM | 2164 | CD | GLU | 1708 | 37.471 | 14.871 | 7.430 | 1.00 | 50.66 |
| ATOM | 2165 | OE1 | GLU | 1708 | 38.199 | 13.986 | 6.909 | 1.00 | 54.73 |
| ATOM | 2166 | OE2 | GLU | 1708 | 37.747 | 16.092 | 7.392 | 1.00 | 52.85 |
| ATOM | 2167 | C | GLU | 1708 | 34.369 | 11.911 | 5.855 | 1.00 | 35.22 |
| ATOM | 2168 | O | GLU | 1708 | 35.035 | 11.045 | 5.260 | 1.00 | 34.04 |
| ATOM | 2169 | N | LEU | 1709 | 33.089 | 11.749 | 6.178 | 1.00 | 33.30 |
| ATOM | 2171 | CA | LEU | 1709 | 32.376 | 10.519 | 5.860 | 1.00 | 31.44 |
| ATOM | 2172 | CB | LEU | 1709 | 30.975 | 10.531 | 6.474 | 1.00 | 26.89 |
| ATOM | 2173 | CG | LEU | 1709 | 30.065 | 9.366 | 6.073 | 1.00 | 26.05 |
| ATOM | 2174 | CD1 | LEU | 1709 | 30.652 | 8.036 | 6.503 | 1.00 | 22.75 |
| ATOM | 2175 | CD2 | LEU | 1709 | 28.717 | 9.574 | 6.597 | 1.00 | 26.15 |
| ATOM | 2176 | C | LEU | 1709 | 32.291 | 10.325 | 4.350 | 1.00 | 31.18 |
| ATOM | 2177 | O | LEU | 1709 | 32.490 | 9.209 | 3.858 | 1.00 | 29.88 |
| ATOM | 2178 | N | PHE | 1710 | 32.011 | 11.408 | 3.623 | 1.00 | 30.16 |
| ATOM | 2180 | CA | PHE | 1710 | 31.915 | 11.333 | 2.169 | 1.00 | 31.64 |
| ATOM | 2181 | CB | PHE | 1710 | 31.658 | 12.710 | 1.567 | 1.00 | 33.44 |
| ATOM | 2182 | CG | PHE | 1710 | 30.287 | 13.231 | 1.827 | 1.00 | 37.78 |
| ATOM | 2183 | CD1 | PHE | 1710 | 29.287 | 12.395 | 2.303 | 1.00 | 41.46 |
| ATOM | 2184 | CD2 | PHE | 1710 | 29.991 | 14.565 | 1.613 | 1.00 | 40.72 |
| ATOM | 2185 | CE1 | PHE | 1710 | 28.012 | 12.882 | 2.566 | 1.00 | 41.30 |
| ATOM | 2186 | CE2 | PHE | 1710 | 28.715 | 15.058 | 1.875 | 1.00 | 42.99 |
| ATOM | 2187 | CZ | PHE | 1710 | 27.725 | 14.208 | 2.354 | 1.00 | 40.95 |
| ATOM | 2188 | C | PHE | 1710 | 33.202 | 10.771 | 1.609 | 1.00 | 32.38 |
| ATOM | 2189 | O | PHE | 1710 | 33.183 | 9.815 | 0.825 | 1.00 | 32.26 |
| ATOM | 2190 | N | LYS | 1711 | 34.310 | 11.336 | 2.085 | 1.00 | 31.26 |
| ATOM | 2192 | CA | LYS | 1711 | 35.664 | 10.971 | 1.697 | 1.00 | 29.73 |
| ATOM | 2193 | CB | LYS | 1711 | 36.642 | 11.932 | 2.379 | 1.00 | 33.49 |
| ATOM | 2194 | CG | LYS | 1711 | 38.103 | 11.716 | 2.042 | 1.00 | 39.79 |
| ATOM | 2195 | CD | LYS | 1711 | 38.981 | 12.731 | 2.755 | 1.00 | 43.35 |
| ATOM | 2196 | CE | LYS | 1711 | 40.413 | 12.686 | 2.238 | 1.00 | 46.23 |
| ATOM | 2197 | NZ | LYS | 1711 | 41.116 | 11.422 | 2.600 | 1.00 | 53.67 |
| ATOM | 2201 | C | LYS | 1711 | 35.999 | 9.501 | 2.015 | 1.00 | 29.34 |
| ATOM | 2202 | O | LYS | 1711 | 36.670 | 8.836 | 1.231 | 1.00 | 28.77 |
| ATOM | 2203 | N | LEU | 1712 | 35.541 | 9.000 | 3.164 | 1.00 | 30.40 |
| ATOM | 2205 | CA | LEU | 1712 | 35.776 | 7.599 | 3.532 | 1.00 | 28.72 |
| ATOM | 2206 | CB | LEU | 1712 | 35.241 | 7.295 | 4.942 | 1.00 | 27.71 |
| ATOM | 2207 | CG | LEU | 1712 | 35.971 | 7.870 | 6.166 | 1.00 | 28.23 |
| ATOM | 2208 | CD1 | LEU | 1712 | 35.186 | 7.593 | 7.440 | 1.00 | 20.80 |
| ATOM | 2209 | CD2 | LEU | 1712 | 37.389 | 7.297 | 6.266 | 1.00 | 27.01 |
| ATOM | 2210 | C | LEU | 1712 | 35.022 | 6.738 | 2.530 | 1.00 | 30.03 |
| ATOM | 2211 | O | LEU | 1712 | 35.571 | 5.796 | 1.957 | 1.00 | 29.28 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2212 | N | LEU | 1713 | 33.752 | 7.073 | 2.325 | 1.00 | 31.98 |
| ATOM | 2214 | CA | LEU | 1713 | 32.904 | 6.339 | 1.403 | 1.00 | 34.30 |
| ATOM | 2215 | CB | LEU | 1713 | 31.467 | 6.872 | 1.447 | 1.00 | 37.65 |
| ATOM | 2216 | CG | LEU | 1713 | 30.663 | 6.450 | 2.686 | 1.00 | 37.06 |
| ATOM | 2217 | CD1 | LEU | 1713 | 29.367 | 7.217 | 2.781 | 1.00 | 36.80 |
| ATOM | 2218 | CD2 | LEU | 1713 | 30.399 | 4.950 | 2.641 | 1.00 | 37.02 |
| ATOM | 2219 | C | LEU | 1713 | 33.451 | 6.344 | -0.011 | 1.00 | 35.45 |
| ATOM | 2220 | O | LEU | 1713 | 33.468 | 5.298 | -0.662 | 1.00 | 38.18 |
| ATOM | 2221 | N | LYS | 1714 | 33.920 | 7.498 | -0.481 | 1.00 | 33.22 |
| ATOM | 2223 | CA | LYS | 1714 | 34.487 | 7.590 | -1.821 | 1.00 | 31.46 |
| ATOM | 2224 | CB | LYS | 1714 | 34.881 | 9.027 | -2.158 | 1.00 | 31.32 |
| ATOM | 2225 | CG | LYS | 1714 | 33.724 | 9.962 | -2.399 | 1.00 | 33.49 |
| ATOM | 2226 | CD | LYS | 1714 | 32.814 | 9.439 | -3.491 | 1.00 | 39.40 |
| ATOM | 2227 | CE | LYS | 1714 | 31.613 | 10.364 | -3.720 | 1.00 | 44.79 |
| ATOM | 2228 | NZ | LYS | 1714 | 30.674 | 9.841 | -4.771 | 1.00 | 50.41 |
| ATOM | 2232 | C | LYS | 1714 | 35.706 | 6.678 | -1.953 | 1.00 | 32.53 |
| ATOM | 2233 | O | LYS | 1714 | 35.998 | 6.155 | -3.025 | 1.00 | 35.46 |
| ATOM | 2234 | N | GLU | 1715 | 36.420 | 6.488 | -0.856 | 1.00 | 33.50 |
| ATOM | 2236 | CA | GLU | 1715 | 37.602 | 5.644 | -0.864 | 1.00 | 34.92 |
| ATOM | 2237 | CB | GLU | 1715 | 38.617 | 6.177 | 0.143 | 1.00 | 37.20 |
| ATOM | 2238 | CG | GLU | 1715 | 39.085 | 7.571 | -0.221 | 1.00 | 44.59 |
| ATOM | 2239 | CD | GLU | 1715 | 39.654 | 8.372 | 0.946 | 1.00 | 51.44 |
| ATOM | 2240 | OE1 | GLU | 1715 | 39.820 | 7.826 | 2.065 | 1.00 | 51.40 |
| ATOM | 2241 | OE2 | GLU | 1715 | 39.930 | 9.573 | 0.726 | 1.00 | 54.23 |
| ATOM | 2242 | C | GLU | 1715 | 37.278 | 4.183 | -0.581 | 1.00 | 35.09 |
| ATOM | 2243 | O | GLU | 1715 | 38.184 | 3.357 | -0.482 | 1.00 | 37.59 |
| ATOM | 2244 | N | GLY | 1716 | 35.991 | 3.866 | -0.455 | 1.00 | 33.79 |
| ATOM | 2246 | CA | GLY | 1716 | 35.576 | 2.498 | -0.197 | 1.00 | 30.96 |
| ATOM | 2247 | C | GLY | 1716 | 35.852 | 1.976 | 1.198 | 1.00 | 29.06 |
| ATOM | 2248 | O | GLY | 1716 | 35.906 | 0.766 | 1.416 | 1.00 | 29.28 |
| ATOM | 2249 | N | HIS | 1717 | 35.995 | 2.879 | 2.155 | 1.00 | 28.16 |
| ATOM | 2251 | CA | HIS | 1717 | 36.282 | 2.489 | 3.532 | 1.00 | 29.80 |
| ATOM | 2252 | CB | HIS | 1717 | 36.534 | 3.743 | 4.378 | 1.00 | 33.13 |
| ATOM | 2253 | CG | HIS | 1717 | 36.794 | 3.469 | 5.826 | 1.00 | 36.22 |
| ATOM | 2254 | CD2 | HIS | 1717 | 37.955 | 3.375 | 6.516 | 1.00 | 35.38 |
| ATOM | 2255 | ND1 | HIS | 1717 | 35.782 | 3.279 | 6.746 | 1.00 | 37.81 |
| ATOM | 2257 | CE1 | HIS | 1717 | 36.309 | 3.080 | 7.942 | 1.00 | 36.97 |
| ATOM | 2258 | NE2 | HIS | 1717 | 37.624 | 3.134 | 7.830 | 1.00 | 35.83 |
| ATOM | 2260 | C | HIS | 1717 | 35.171 | 1.645 | 4.153 | 1.00 | 29.26 |
| ATOM | 2261 | O | HIS | 1717 | 33.987 | 1.900 | 3.940 | 1.00 | 31.43 |
| ATOM | 2262 | N | ARG | 1718 | 35.571 | 0.666 | 4.955 | 1.00 | 28.11 |
| ATOM | 2264 | CA | ARG | 1718 | 34.632 | -0.212 | 5.640 | 1.00 | 30.67 |
| ATOM | 2265 | CB | ARG | 1718 | 34.592 | -1.583 | 4.973 | 1.00 | 27.32 |
| ATOM | 2266 | CG | ARG | 1718 | 34.058 | -1.586 | 3.557 | 1.00 | 28.77 |
| ATOM | 2267 | CD | ARG | 1718 | 32.609 | -1.111 | 3.484 | 1.00 | 28.84 |
| ATOM | 2268 | NE | ARG | 1718 | 32.032 | -1.167 | 2.131 | 1.00 | 24.96 |
| ATOM | 2270 | CZ | ARG | 1718 | 32.141 | -0.206 | 1.204 | 1.00 | 23.90 |
| ATOM | 2271 | NH1 | ARG | 1718 | 32.824 | 0.912 | 1.454 | 1.00 | 20.04 |
| ATOM | 2274 | NH2 | ARG | 1718 | 31.513 | -0.338 | 0.045 | 1.00 | 20.04 |
| ATOM | 2277 | C | ARG | 1718 | 35.091 | -0.350 | 7.101 | 1.00 | 33.92 |
| ATOM | 2278 | O | ARG | 1718 | 36.300 | -0.449 | 7.377 | 1.00 | 36.48 |
| ATOM | 2279 | N | MET | 1719 | 34.134 | -0.355 | 8.028 | 1.00 | 33.22 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2281 | CA | MET | 1719 | 34.428 | -0.459 | 9.448 | 1.00 | 32.33 |
| ATOM | 2282 | CB | MET | 1719 | 33.148 | -0.285 | 10.277 | 1.00 | 34.72 |
| ATOM | 2283 | CG | MET | 1719 | 32.454 | 1.066 | 10.076 | 1.00 | 35.04 |
| ATOM | 2284 | SD | MET | 1719 | 31.025 | 1.447 | 11.141 | 1.00 | 34.06 |
| ATOM | 2285 | CE | MET | 1719 | 29.757 | 0.470 | 10.409 | 1.00 | 33.14 |
| ATOM | 2286 | C | MET | 1719 | 35.068 | -1.797 | 9.747 | 1.00 | 35.53 |
| ATOM | 2287 | O | MET | 1719 | 34.896 | -2.756 | 8.991 | 1.00 | 35.48 |
| ATOM | 2288 | N | ASP | 1720 | 35.826 | -1.843 | 10.840 | 1.00 | 38.65 |
| ATOM | 2290 | CA | ASP | 1720 | 36.521 | -3.049 | 11.281 | 1.00 | 39.03 |
| ATOM | 2291 | CB | ASP | 1720 | 37.659 | -2.678 | 12.237 | 1.00 | 43.11 |
| ATOM | 2292 | CG | ASP | 1720 | 38.743 | -1.846 | 11.569 | 1.00 | 46.69 |
| ATOM | 2293 | OD1 | ASP | 1720 | 38.587 | -1.536 | 10.364 | 1.00 | 54.08 |
| ATOM | 2294 | OD2 | ASP | 1720 | 39.750 | -1.503 | 12.239 | 1.00 | 45.93 |
| ATOM | 2295 | C | ASP | 1720 | 35.580 | -4.023 | 11.972 | 1.00 | 38.50 |
| ATOM | 2296 | O | ASP | 1720 | 34.554 | -3.617 | 12.528 | 1.00 | 37.73 |
| ATOM | 2297 | N | LYS | 1721 | 35.961 | -5.298 | 11.981 | 1.00 | 38.10 |
| ATOM | 2299 | CA | LYS | 1721 | 35.151 | -6.339 | 12.600 | 1.00 | 38.12 |
| ATOM | 2300 | CB | LYS | 1721 | 35.727 | -7.733 | 12.323 | 1.00 | 38.20 |
| ATOM | 2301 | CG | LYS | 1721 | 34.825 | -8.858 | 12.825 | 1.00 | 38.48 |
| ATOM | 2302 | CD | LYS | 1721 | 35.375 | -10.238 | 12.543 | 1.00 | 37.49 |
| ATOM | 2303 | CE | LYS | 1721 | 36.320 | -10.691 | 13.625 | 1.00 | 39.11 |
| ATOM | 2304 | NZ | LYS | 1721 | 36.448 | -12.167 | 13.628 | 1.00 | 40.75 |
| ATOM | 2308 | C | LYS | 1721 | 35.092 | -6.142 | 14.091 | 1.00 | 40.24 |
| ATOM | 2309 | O | LYS | 1721 | 36.136 | -6.032 | 14.739 | 1.00 | 42.70 |
| ATOM | 2310 | N | PRO | 1722 | 33.875 | -6.082 | 14.658 | 1.00 | 41.23 |
| ATOM | 2311 | CD | PRO | 1722 | 32.547 | -6.153 | 14.019 | 1.00 | 38.63 |
| ATOM | 2312 | CA | PRO | 1722 | 33.743 | -5.901 | 16.104 | 1.00 | 41.71 |
| ATOM | 2313 | CB | PRO | 1722 | 32.223 | -5.957 | 16.306 | 1.00 | 38.90 |
| ATOM | 2314 | CG | PRO | 1722 | 31.679 | -5.442 | 15.016 | 1.00 | 34.19 |
| ATOM | 2315 | C | PRO | 1722 | 34.418 | -7.079 | 16.819 | 1.00 | 43.96 |
| ATOM | 2316 | O | PRO | 1722 | 34.542 | -8.174 | 16.250 | 1.00 | 43.02 |
| ATOM | 2317 | N | SER | 1723 | 34.915 | -6.860 | 18.028 | 1.00 | 46.76 |
| ATOM | 2319 | CA | SER | 1723 | 35.493 | -7.973 | 18.747 | 1.00 | 50.74 |
| ATOM | 2320 | CB | SER | 1723 | 36.265 | -7.500 | 19.980 | 1.00 | 49.47 |
| ATOM | 2321 | OG | SER | 1723 | 35.400 | -7.130 | 21.035 | 1.00 | 53.87 |
| ATOM | 2323 | C | SER | 1723 | 34.259 | -8.782 | 19.143 | 1.00 | 53.24 |
| ATOM | 2324 | O | SER | 1723 | 33.136 | -8.259 | 19.130 | 1.00 | 53.97 |
| ATOM | 2325 | N | ASN | 1724 | 34.443 | -10.064 | 19.426 | 1.00 | 56.59 |
| ATOM | 2327 | CA | ASN | 1724 | 33.316 | -10.899 | 19.825 | 1.00 | 59.55 |
| ATOM | 2328 | CB | ASN | 1724 | 32.739 | -10.386 | 21.162 | 1.00 | 66.12 |
| ATOM | 2329 | CG | ASN | 1724 | 33.824 | -10.128 | 22.213 | 1.00 | 71.34 |
| ATOM | 2330 | OD1 | ASN | 1724 | 34.661 | -10.990 | 22.485 | 1.00 | 73.38 |
| ATOM | 2331 | ND2 | ASN | 1724 | 33.831 | -8.926 | 22.779 | 1.00 | 74.19 |
| ATOM | 2334 | C | ASN | 1724 | 32.256 | -10.900 | 18.711 | 1.00 | 57.31 |
| ATOM | 2335 | O | ASN | 1724 | 31.073 | -10.662 | 18.940 | 1.00 | 59.27 |
| ATOM | 2336 | N | CYS | 1725 | 32.723 | -11.132 | 17.493 | 1.00 | 54.50 |
| ATOM | 2338 | CA | CYS | 1725 | 31.881 | -11.203 | 16.300 | 1.00 | 50.89 |
| ATOM | 2339 | CB | CYS | 1725 | 31.827 | -9.848 | 15.576 | 1.00 | 50.09 |
| ATOM | 2340 | SG | CYS | 1725 | 30.893 | -9.833 | 14.006 | 1.00 | 44.81 |
| ATOM | 2341 | C | CYS | 1725 | 32.596 | -12.235 | 15.439 | 1.00 | 47.28 |
| ATOM | 2342 | O | CYS | 1725 | 33.820 | -12.172 | 15.288 | 1.00 | 48.97 |
| ATOM | 2343 | N | THR | 1726 | 31.863 | -13.229 | 14.950 | 1.00 | 42.60 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2345 | CA | THR | 1726 | 32.472 | -14.275 | 14.139 | 1.00 | 39.22 |
| ATOM | 2346 | CB | THR | 1726 | 31.520 | -15.494 | 13.984 | 1.00 | 36.36 |
| ATOM | 2347 | OG1 | THR | 1726 | 30.290 | -15.087 | 13.363 | 1.00 | 36.62 |
| ATOM | 2349 | CG2 | THR | 1726 | 31.210 | -16.084 | 15.326 | 1.00 | 33.12 |
| ATOM | 2350 | C | THR | 1726 | 32.858 | -13.748 | 12.776 | 1.00 | 37.99 |
| ATOM | 2351 | O | THR | 1726 | 32.373 | -12.704 | 12.357 | 1.00 | 39.57 |
| ATOM | 2352 | N | ASN | 1727 | 33.724 | -14.473 | 12.080 | 1.00 | 37.02 |
| ATOM | 2354 | CA | ASN | 1727 | 34.133 | -14.044 | 10.742 | 1.00 | 38.17 |
| ATOM | 2355 | CB | ASN | 1727 | 35.290 | -14.880 | 10.221 | 1.00 | 40.63 |
| ATOM | 2356 | CG | ASN | 1727 | 36.580 | -14.593 | 10.953 | 1.00 | 44.79 |
| ATOM | 2357 | OD1 | ASN | 1727 | 37.188 | -13.539 | 10.781 | 1.00 | 46.57 |
| ATOM | 2358 | ND2 | ASN | 1727 | 37.010 | -15.536 | 11.778 | 1.00 | 48.30 |
| ATOM | 2361 | C | ASN | 1727 | 32.958 | -14.159 | 9.786 | 1.00 | 38.22 |
| ATOM | 2362 | O | ASN | 1727 | 32.883 | -13.431 | 8.793 | 1.00 | 39.53 |
| ATOM | 2363 | N | GLU | 1728 | 32.041 | -15.076 | 10.093 | 1.00 | 37.33 |
| ATOM | 2365 | CA | GLU | 1728 | 30.854 | -15.312 | 9.273 | 1.00 | 34.24 |
| ATOM | 2366 | CB | GLU | 1728 | 30.109 | -16.551 | 9.765 | 1.00 | 32.82 |
| ATOM | 2367 | CG | GLU | 1728 | 28.973 | -17.000 | 8.855 | 1.00 | 35.84 |
| ATOM | 2368 | CD | GLU | 1728 | 28.329 | -18.306 | 9.297 | 1.00 | 42.16 |
| ATOM | 2369 | OE1 | GLU | 1728 | 28.409 | -18.633 | 10.504 | 1.00 | 46.78 |
| ATOM | 2370 | OE2 | GLU | 1728 | 27.734 | -18.996 | 8.440 | 1.00 | 38.81 |
| ATOM | 2371 | C | GLU | 1728 | 29.925 | -14.104 | 9.313 | 1.00 | 33.05 |
| ATOM | 2372 | O | GLU | 1728 | 29.521 | -13.574 | 8.272 | 1.00 | 29.58 |
| ATOM | 2373 | N | LEU | 1729 | 29.608 | -13.671 | 10.527 | 1.00 | 32.09 |
| ATOM | 2375 | CA | LEU | 1729 | 28.741 | -12.530 | 10.710 | 1.00 | 32.45 |
| ATOM | 2376 | CB | LEU | 1729 | 28.351 | -12.389 | 12.170 | 1.00 | 32.64 |
| ATOM | 2377 | CG | LEU | 1729 | 27.311 | -13.431 | 12.575 | 1.00 | 34.65 |
| ATOM | 2378 | CD1 | LEU | 1729 | 27.131 | -13.388 | 14.089 | 1.00 | 37.18 |
| ATOM | 2379 | CD2 | LEU | 1729 | 25.988 | -13.167 | 11.842 | 1.00 | 27.77 |
| ATOM | 2380 | C | LEU | 1729 | 29.359 | -11.252 | 10.175 | 1.00 | 32.68 |
| ATOM | 2381 | O | LEU | 1729 | 28.638 | -10.367 | 9.693 | 1.00 | 31.97 |
| ATOM | 2382 | N | TYR | 1730 | 30.688 | -11.143 | 10.251 | 1.00 | 31.70 |
| ATOM | 2384 | CA | TYR | 1730 | 31.378 | -9.959 | 9.734 | 1.00 | 30.19 |
| ATOM | 2385 | CB | TYR | 1730 | 32.849 | -9.940 | 10.154 | 1.00 | 27.88 |
| ATOM | 2386 | CG | TYR | 1730 | 33.591 | -8.723 | 9.649 | 1.00 | 26.63 |
| ATOM | 2387 | CD1 | TYR | 1730 | 33.093 | -7.449 | 9.879 | 1.00 | 27.37 |
| ATOM | 2388 | CE1 | TYR | 1730 | 33.725 | -6.324 | 9.378 | 1.00 | 27.56 |
| ATOM | 2389 | CD2 | TYR | 1730 | 34.759 | -8.849 | 8.904 | 1.00 | 24.07 |
| ATOM | 2390 | CE2 | TYR | 1730 | 35.408 | -7.724 | 8.393 | 1.00 | 24.81 |
| ATOM | 2391 | CZ | TYR | 1730 | 34.882 | -6.462 | 8.631 | 1.00 | 28.56 |
| ATOM | 2392 | OH | TYR | 1730 | 35.473 | -5.316 | 8.111 | 1.00 | 29.08 |
| ATOM | 2394 | C | TYR | 1730 | 31.287 | -9.962 | 8.208 | 1.00 | 29.50 |
| ATOM | 2395 | O | TYR | 1730 | 31.062 | -8.928 | 7.585 | 1.00 | 29.16 |
| ATOM | 2396 | N | MET | 1731 | 31.443 | -11.139 | 7.623 | 1.00 | 31.05 |
| ATOM | 2398 | CA | MET | 1731 | 31.366 | -11.313 | 6.187 | 1.00 | 34.59 |
| ATOM | 2399 | CB | MET | 1731 | 31.611 | -12.779 | 5.840 | 1.00 | 41.42 |
| ATOM | 2400 | CG | MET | 1731 | 31.315 | -13.149 | 4.403 | 1.00 | 52.20 |
| ATOM | 2401 | SD | MET | 1731 | 31.801 | -14.840 | 3.994 | 1.00 | 64.38 |
| ATOM | 2402 | CE | MET | 1731 | 32.926 | -14.502 | 2.606 | 1.00 | 63.03 |
| ATOM | 2403 | C | MET | 1731 | 29.992 | -10.869 | 5.695 | 1.00 | 34.53 |
| ATOM | 2404 | O | MET | 1731 | 29.863 | -10.268 | 4.619 | 1.00 | 35.08 |
| ATOM | 2405 | N | MET | 1732 | 28.971 | -11.153 | 6.501 | 1.00 | 33.32 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2407 | CA | MET | 1732 | 27.594 | -10.770 | 6.194 | 1.00 | 31.78 |
| ATOM | 2408 | CB | MET | 1732 | 26.634 | -11.346 | 7.236 | 1.00 | 30.42 |
| ATOM | 2409 | CG | MET | 1732 | 25.172 | -11.071 | 6.938 | 1.00 | 30.28 |
| ATOM | 2410 | SD | MET | 1732 | 24.071 | -11.709 | 8.183 | 1.00 | 27.41 |
| ATOM | 2411 | CE | MET | 1732 | 23.738 | -13.369 | 7.471 | 1.00 | 22.35 |
| ATOM | 2412 | C | MET | 1732 | 27.484 | -9.243 | 6.158 | 1.00 | 31.10 |
| ATOM | 2413 | O | MET | 1732 | 26.794 | -8.680 | 5.303 | 1.00 | 31.08 |
| ATOM | 2414 | N | MET | 1733 | 28.139 | -8.586 | 7.114 | 1.00 | 31.22 |
| ATOM | 2416 | CA | MET | 1733 | 28.161 | -7.128 | 7.189 | 1.00 | 30.93 |
| ATOM | 2417 | CB | MET | 1733 | 29.001 | -6.665 | 8.376 | 1.00 | 31.91 |
| ATOM | 2418 | CG | MET | 1733 | 28.368 | -6.906 | 9.710 | 1.00 | 33.63 |
| ATOM | 2419 | SD | MET | 1733 | 29.375 | -6.210 | 11.021 | 1.00 | 34.53 |
| ATOM | 2420 | CE | MET | 1733 | 29.106 | -7.395 | 12.280 | 1.00 | 34.12 |
| ATOM | 2421 | C | MET | 1733 | 28.830 | -6.623 | 5.921 | 1.00 | 32.49 |
| ATOM | 2422 | O | MET | 1733 | 28.357 | -5.682 | 5.281 | 1.00 | 33.61 |
| ATOM | 2423 | N | ARG | 1734 | 29.932 | -7.269 | 5.551 | 1.00 | 32.11 |
| ATOM | 2425 | CA | ARG | 1734 | 30.673 | -6.889 | 4.355 | 1.00 | 31.13 |
| ATOM | 2426 | CB | ARG | 1734 | 32.012 | -7.623 | 4.308 | 1.00 | 28.68 |
| ATOM | 2427 | CG | ARG | 1734 | 32.953 | -7.267 | 5.451 | 1.00 | 27.19 |
| ATOM | 2428 | CD | ARG | 1734 | 33.159 | -5.766 | 5.558 | 1.00 | 26.80 |
| ATOM | 2429 | NE | ARG | 1734 | 33.864 | -5.243 | 4.393 | 1.00 | 35.67 |
| ATOM | 2431 | CZ | ARG | 1734 | 35.187 | -5.305 | 4.223 | 1.00 | 38.03 |
| ATOM | 2432 | NH1 | ARG | 1734 | 35.967 | -5.861 | 5.148 | 1.00 | 38.07 |
| ATOM | 2435 | NH2 | ARG | 1734 | 35.729 | -4.850 | 3.094 | 1.00 | 38.87 |
| ATOM | 2438 | C | ARG | 1734 | 29.873 | -7.098 | 3.065 | 1.00 | 29.53 |
| ATOM | 2439 | O | ARG | 1734 | 30.029 | -6.334 | 2.121 | 1.00 | 29.11 |
| ATOM | 2440 | N | ASP | 1735 | 29.036 | -8.137 | 3.025 | 1.00 | 29.48 |
| ATOM | 2442 | CA | ASP | 1735 | 28.193 | -8.412 | 1.859 | 1.00 | 26.82 |
| ATOM | 2443 | CB | ASP | 1735 | 27.591 | -9.811 | 1.933 | 1.00 | 30.25 |
| ATOM | 2444 | CG | ASP | 1735 | 28.632 | -10.895 | 1.773 | 1.00 | 35.13 |
| ATOM | 2445 | OD1 | ASP | 1735 | 29.626 | -10.645 | 1.052 | 1.00 | 35.19 |
| ATOM | 2446 | OD2 | ASP | 1735 | 28.458 | -11.990 | 2.366 | 1.00 | 39.35 |
| ATOM | 2447 | C | ASP | 1735 | 27.082 | -7.375 | 1.760 | 1.00 | 23.88 |
| ATOM | 2448 | O | ASP | 1735 | 26.692 | -6.992 | 0.656 | 1.00 | 24.83 |
| ATOM | 2449 | N | CYS | 1736 | 26.574 | -6.929 | 2.913 | 1.00 | 22.13 |
| ATOM | 2451 | CA | CYS | 1736 | 25.538 | -5.887 | 2.965 | 1.00 | 21.74 |
| ATOM | 2452 | CB | CYS | 1736 | 25.005 | -5.692 | 4.401 | 1.00 | 20.46 |
| ATOM | 2453 | SG | CYS | 1736 | 23.978 | -7.013 | 5.053 | 1.00 | 19.59 |
| ATOM | 2454 | C | CYS | 1736 | 26.104 | -4.542 | 2.456 | 1.00 | 20.51 |
| ATOM | 2455 | O | CYS | 1736 | 25.377 | -3.732 | 1.887 | 1.00 | 16.07 |
| ATOM | 2456 | N | TRP | 1737 | 27.401 | -4.325 | 2.670 | 1.00 | 21.58 |
| ATOM | 2458 | CA | TRP | 1737 | 28.080 | -3.113 | 2.248 | 1.00 | 20.57 |
| ATOM | 2459 | CB | TRP | 1737 | 29.107 | -2.682 | 3.291 | 1.00 | 17.02 |
| ATOM | 2460 | CG | TRP | 1737 | 28.558 | -2.415 | 4.654 | 1.00 | 20.35 |
| ATOM | 2461 | CD2 | TRP | 1737 | 29.254 | -2.564 | 5.897 | 1.00 | 20.42 |
| ATOM | 2462 | CE2 | TRP | 1737 | 28.387 | -2.122 | 6.923 | 1.00 | 21.18 |
| ATOM | 2463 | CE3 | TRP | 1737 | 30.538 | -3.027 | 6.243 | 1.00 | 21.60 |
| ATOM | 2464 | CD1 | TRP | 1737 | 27.317 | -1.914 | 4.970 | 1.00 | 19.86 |
| ATOM | 2465 | NE1 | TRP | 1737 | 27.210 | -1.732 | 6.328 | 1.00 | 21.03 |
| ATOM | 2467 | CZ2 | TRP | 1737 | 28.760 | -2.125 | 8.276 | 1.00 | 21.70 |
| ATOM | 2468 | CZ3 | TRP | 1737 | 30.910 | -3.031 | 7.594 | 1.00 | 21.73 |
| ATOM | 2469 | CH2 | TRP | 1737 | 30.025 | -2.584 | 8.588 | 1.00 | 23.06 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2470 | C | TRP | 1737 | 28.770 | -3.281 | 0.899 | 1.00 | 24.98 |
| ATOM | 2471 | O | TRP | 1737 | 29.758 | -2.607 | 0.610 | 1.00 | 25.84 |
| ATOM | 2472 | N | HIS | 1738 | 28.269 | -4.185 | 0.063 | 1.00 | 27.61 |
| ATOM | 2474 | CA | HIS | 1738 | 28.885 | -4.352 | -1.243 | 1.00 | 25.81 |
| ATOM | 2475 | CB | HIS | 1738 | 28.263 | -5.522 | -2.013 | 1.00 | 24.74 |
| ATOM | 2476 | CG | HIS | 1738 | 29.105 | -6.005 | -3.162 | 1.00 | 26.07 |
| ATOM | 2477 | CD2 | HIS | 1738 | 29.599 | -5.353 | -4.246 | 1.00 | 25.45 |
| ATOM | 2478 | ND1 | HIS | 1738 | 29.571 | -7.299 | -3.252 | 1.00 | 24.60 |
| ATOM | 2480 | CE1 | HIS | 1738 | 30.320 | -7.422 | -4.333 | 1.00 | 24.62 |
| ATOM | 2481 | NE2 | HIS | 1738 | 30.352 | -6.253 | -4.954 | 1.00 | 23.97 |
| ATOM | 2483 | C | HIS | 1738 | 28.734 | -3.034 | -2.017 | 1.00 | 26.41 |
| ATOM | 2484 | O | HIS | 1738 | 27.705 | -2.350 | -1.931 | 1.00 | 25.20 |
| ATOM | 2485 | N | ALA | 1739 | 29.792 | -2.658 | -2.727 | 1.00 | 26.45 |
| ATOM | 2487 | CA | ALA | 1739 | 29.829 | -1.437 | -3.517 | 1.00 | 25.61 |
| ATOM | 2488 | CB | ALA | 1739 | 31.193 | -1.285 | -4.117 | 1.00 | 25.87 |
| ATOM | 2489 | C | ALA | 1739 | 28.765 | -1.418 | -4.617 | 1.00 | 26.67 |
| ATOM | 2490 | O | ALA | 1739 | 28.207 | -0.367 | -4.930 | 1.00 | 28.28 |
| ATOM | 2491 | N | VAL | 1740 | 28.529 | -2.573 | -5.235 | 1.00 | 25.10 |
| ATOM | 2493 | CA | VAL | 1740 | 27.526 | -2.706 | -6.292 | 1.00 | 24.14 |
| ATOM | 2494 | CB | VAL | 1740 | 27.969 | -3.737 | -7.378 | 1.00 | 24.27 |
| ATOM | 2495 | CG1 | VAL | 1740 | 26.979 | -3.792 | -8.503 | 1.00 | 20.03 |
| ATOM | 2496 | CG2 | VAL | 1740 | 29.331 | -3.375 | -7.926 | 1.00 | 26.74 |
| ATOM | 2497 | C | VAL | 1740 | 26.234 | -3.196 | -5.639 | 1.00 | 23.91 |
| ATOM | 2498 | O | VAL | 1740 | 26.173 | -4.349 | -5.175 | 1.00 | 26.37 |
| ATOM | 2499 | N | PRO | 1741 | 25.173 | -2.357 | -5.653 | 1.00 | 24.55 |
| ATOM | 2500 | CD | PRO | 1741 | 25.096 | -1.065 | -6.369 | 1.00 | 17.73 |
| ATOM | 2501 | CA | PRO | 1741 | 23.868 | -2.686 | -5.058 | 1.00 | 22.27 |
| ATOM | 2502 | CB | PRO | 1741 | 22.979 | -1.536 | -5.545 | 1.00 | 17.82 |
| ATOM | 2503 | CG | PRO | 1741 | 23.925 | -0.410 | -5.710 | 1.00 | 13.27 |
| ATOM | 2504 | C | PRO | 1741 | 23.275 | -4.057 | -5.418 | 1.00 | 24.04 |
| ATOM | 2505 | O | PRO | 1741 | 22.735 | -4.748 | -4.548 | 1.00 | 25.86 |
| ATOM | 2506 | N | SER | 1742 | 23.431 | -4.471 | -6.674 | 1.00 | 24.30 |
| ATOM | 2508 | CA | SER | 1742 | 22.888 | -5.745 | -7.167 | 1.00 | 24.42 |
| ATOM | 2509 | CB | SER | 1742 | 22.986 | -5.819 | -8.696 | 1.00 | 23.95 |
| ATOM | 2510 | OG | SER | 1742 | 24.334 | -5.784 | -9.131 | 1.00 | 22.98 |
| ATOM | 2512 | C | SER | 1742 | 23.553 | -6.978 | -6.589 | 1.00 | 25.20 |
| ATOM | 2513 | O | SER | 1742 | 22.994 | -8.085 | -6.677 | 1.00 | 23.68 |
| ATOM | 2514 | N | GLN | 1743 | 24.753 | -6.793 | -6.037 | 1.00 | 25.46 |
| ATOM | 2516 | CA | GLN | 1743 | 25.504 | -7.910 | -5.485 | 1.00 | 25.64 |
| ATOM | 2517 | CB | GLN | 1743 | 26.993 | -7.773 | -5.807 | 1.00 | 24.02 |
| ATOM | 2518 | CG | GLN | 1743 | 27.263 | -7.768 | -7.295 | 1.00 | 22.75 |
| ATOM | 2519 | CD | GLN | 1743 | 26.585 | -8.938 | -8.014 | 1.00 | 26.21 |
| ATOM | 2520 | OE1 | GLN | 1743 | 26.999 | -10.087 | -7.864 | 1.00 | 28.67 |
| ATOM | 2521 | NE2 | GLN | 1743 | 25.535 | -8.649 | -8.787 | 1.00 | 21.57 |
| ATOM | 2524 | C | GLN | 1743 | 25.270 | -8.148 | -4.007 | 1.00 | 24.86 |
| ATOM | 2525 | O | GLN | 1743 | 25.685 | -9.173 | -3.456 | 1.00 | 25.24 |
| ATOM | 2526 | N | ARG | 1744 | 24.525 | -7.244 | -3.389 | 1.00 | 23.38 |
| ATOM | 2528 | CA | ARG | 1744 | 24.230 | -7.376 | -1.976 | 1.00 | 22.41 |
| ATOM | 2529 | CB | ARG | 1744 | 23.727 | -6.055 | -1.415 | 1.00 | 22.24 |
| ATOM | 2530 | CG | ARG | 1744 | 24.718 | -4.909 | -1.523 | 1.00 | 22.53 |
| ATOM | 2531 | CD | ARG | 1744 | 24.084 | -3.577 | -1.134 | 1.00 | 19.82 |
| ATOM | 2532 | NE | ARG | 1744 | 24.963 | -2.475 | -1.517 | 1.00 | 22.51 |

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ATOM   2534  CZ  ARG  1744      24.592  -1.201  -1.663  1.00 22.92
ATOM   2535  NH1 ARG  1744      23.332  -0.814  -1.458  1.00 18.28
ATOM   2538  NH2 ARG  1744      25.491  -0.310  -2.060  1.00 22.15
ATOM   2541  C   ARG  1744      23.163  -8.458  -1.833  1.00 24.61
ATOM   2542  O   ARG  1744      22.428  -8.755  -2.786  1.00 26.94
ATOM   2543  N   PRO  1745      23.143  -9.155  -0.688  1.00 23.21
ATOM   2544  CD  PRO  1745      24.052  -9.107   0.470  1.00 22.38
ATOM   2545  CA  PRO  1745      22.129 -10.190  -0.522  1.00 22.24
ATOM   2546  CB  PRO  1745      22.623 -10.942   0.711  1.00 21.13
ATOM   2547  CG  PRO  1745      23.286  -9.864   1.504  1.00 20.24
ATOM   2548  C   PRO  1745      20.800  -9.506  -0.256  1.00 23.11
ATOM   2549  O   PRO  1745      20.743  -8.300   0.020  1.00 25.93
ATOM   2550  N   THR  1746      19.724 -10.256  -0.373  1.00 20.82
ATOM   2552  CA  THR  1746      18.420  -9.697  -0.112  1.00 20.47
ATOM   2553  CB  THR  1746      17.386 -10.342  -1.041  1.00 18.61
ATOM   2554  OG1 THR  1746      17.382 -11.755  -0.822  1.00 21.86
ATOM   2556  CG2 THR  1746      17.746 -10.078  -2.487  1.00 21.13
ATOM   2557  C   THR  1746      18.060  -9.970   1.344  1.00 20.84
ATOM   2558  O   THR  1746      18.787 -10.674   2.055  1.00 22.08
ATOM   2559  N   PHE  1747      16.953  -9.406   1.810  1.00 21.58
ATOM   2561  CA  PHE  1747      16.536  -9.675   3.178  1.00 21.15
ATOM   2562  CB  PHE  1747      15.442  -8.710   3.613  1.00 20.34
ATOM   2563  CG  PHE  1747      15.961  -7.350   3.982  1.00 23.18
ATOM   2564  CD1 PHE  1747      16.729  -7.170   5.130  1.00 22.26
ATOM   2565  CD2 PHE  1747      15.668  -6.240   3.196  1.00 23.41
ATOM   2566  CE1 PHE  1747      17.186  -5.909   5.484  1.00 17.31
ATOM   2567  CE2 PHE  1747      16.124  -4.967   3.548  1.00 17.93
ATOM   2568  CZ  PHE  1747      16.883  -4.809   4.696  1.00 19.06
ATOM   2569  C   PHE  1747      16.062 -11.124   3.217  1.00 21.61
ATOM   2570  O   PHE  1747      16.248 -11.823   4.212  1.00 22.19
ATOM   2571  N   LYS  1748      15.490 -11.588   2.111  1.00 22.00
ATOM   2573  CA  LYS  1748      15.048 -12.973   2.009  1.00 24.34
ATOM   2574  CB  LYS  1748      14.471 -13.227   0.621  1.00 23.61
ATOM   2575  CG  LYS  1748      14.050 -14.663   0.416  1.00 27.45
ATOM   2576  CD  LYS  1748      13.633 -14.932  -0.998  1.00 28.97
ATOM   2577  CE  LYS  1748      13.244 -16.394  -1.163  1.00 35.95
ATOM   2578  NZ  LYS  1748      12.213 -16.795  -0.153  1.00 41.69
ATOM   2582  C   LYS  1748      16.257 -13.907   2.264  1.00 27.58
ATOM   2583  O   LYS  1748      16.161 -14.863   3.034  1.00 29.73
ATOM   2584  N   GLN  1749      17.397 -13.604   1.640  1.00 25.88
ATOM   2586  CA  GLN  1749      18.617 -14.394   1.804  1.00 23.72
ATOM   2587  CB  GLN  1749      19.692 -13.925   0.837  1.00 27.00
ATOM   2588  CG  GLN  1749      19.338 -13.954  -0.628  1.00 32.28
ATOM   2589  CD  GLN  1749      20.442 -13.331  -1.477  1.00 36.35
ATOM   2590  OE1 GLN  1749      20.175 -12.528  -2.368  1.00 37.63
ATOM   2591  NE2 GLN  1749      21.699 -13.702  -1.194  1.00 38.60
ATOM   2594  C   GLN  1749      19.177 -14.266   3.212  1.00 23.44
ATOM   2595  O   GLN  1749      19.586 -15.260   3.826  1.00 23.52
ATOM   2596  N   LEU  1750      19.267 -13.035   3.703  1.00 21.73
ATOM   2598  CA  LEU  1750      19.787 -12.796   5.054  1.00 20.90
ATOM   2599  CB  LEU  1750      19.752 -11.308   5.359  1.00 18.60
ATOM   2600  CG  LEU  1750      20.654 -10.439   4.485  1.00 16.53
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2601 | CD1 | LEU | 1750 | 20.190 | -8.979 | 4.579 | 1.00 | 13.28 |
| ATOM | 2602 | CD2 | LEU | 1750 | 22.100 | -10.612 | 4.939 | 1.00 | 14.74 |
| ATOM | 2603 | C | LEU | 1750 | 18.982 | -13.548 | 6.108 | 1.00 | 21.25 |
| ATOM | 2604 | O | LEU | 1750 | 19.534 | -14.056 | 7.084 | 1.00 | 21.26 |
| ATOM | 2605 | N | VAL | 1751 | 17.671 | -13.607 | 5.917 | 1.00 | 21.64 |
| ATOM | 2607 | CA | VAL | 1751 | 16.793 | -14.289 | 6.845 | 1.00 | 21.21 |
| ATOM | 2608 | CB | VAL | 1751 | 15.353 | -14.072 | 6.432 | 1.00 | 19.03 |
| ATOM | 2609 | CG1 | VAL | 1751 | 14.453 | -14.970 | 7.220 | 1.00 | 23.34 |
| ATOM | 2610 | CG2 | VAL | 1751 | 14.978 | -12.648 | 6.684 | 1.00 | 22.78 |
| ATOM | 2611 | C | VAL | 1751 | 17.127 | -15.774 | 6.925 | 1.00 | 25.56 |
| ATOM | 2612 | O | VAL | 1751 | 17.111 | -16.369 | 8.007 | 1.00 | 25.61 |
| ATOM | 2613 | N | GLU | 1752 | 17.418 | -16.381 | 5.778 | 1.00 | 28.61 |
| ATOM | 2615 | CA | GLU | 1752 | 17.773 | -17.789 | 5.755 | 1.00 | 32.38 |
| ATOM | 2616 | CB | GLU | 1752 | 17.765 | -18.317 | 4.321 | 1.00 | 37.26 |
| ATOM | 2617 | CG | GLU | 1752 | 16.399 | -18.218 | 3.651 | 1.00 | 44.76 |
| ATOM | 2618 | CD | GLU | 1752 | 16.394 | -18.742 | 2.219 | 1.00 | 50.37 |
| ATOM | 2619 | OE1 | GLU | 1752 | 15.397 | -18.495 | 1.497 | 1.00 | 52.52 |
| ATOM | 2620 | OE2 | GLU | 1752 | 17.377 | -19.410 | 1.822 | 1.00 | 51.96 |
| ATOM | 2621 | C | GLU | 1752 | 19.140 | -17.984 | 6.405 | 1.00 | 32.27 |
| ATOM | 2622 | O | GLU | 1752 | 19.330 | -18.878 | 7.237 | 1.00 | 31.18 |
| ATOM | 2623 | N | ASP | 1753 | 20.069 | -17.096 | 6.083 | 1.00 | 33.20 |
| ATOM | 2625 | CA | ASP | 1753 | 21.411 | -17.174 | 6.647 | 1.00 | 35.13 |
| ATOM | 2626 | CB | ASP | 1753 | 22.341 | -16.144 | 5.998 | 1.00 | 37.80 |
| ATOM | 2627 | CG | ASP | 1753 | 22.498 | -16.358 | 4.502 | 1.00 | 41.13 |
| ATOM | 2628 | OD1 | ASP | 1753 | 22.222 | -17.470 | 4.007 | 1.00 | 43.01 |
| ATOM | 2629 | OD2 | ASP | 1753 | 22.908 | -15.401 | 3.811 | 1.00 | 44.26 |
| ATOM | 2630 | C | ASP | 1753 | 21.378 | -16.986 | 8.163 | 1.00 | 33.84 |
| ATOM | 2631 | O | ASP | 1753 | 21.971 | -17.773 | 8.901 | 1.00 | 36.22 |
| ATOM | 2632 | N | LEU | 1754 | 20.652 | -15.978 | 8.633 | 1.00 | 30.73 |
| ATOM | 2634 | CA | LEU | 1754 | 20.568 | -15.730 | 10.070 | 1.00 | 28.51 |
| ATOM | 2635 | CB | LEU | 1754 | 19.881 | -14.394 | 10.355 | 1.00 | 25.20 |
| ATOM | 2636 | CG | LEU | 1754 | 20.810 | -13.225 | 10.016 | 1.00 | 26.72 |
| ATOM | 2637 | CD1 | LEU | 1754 | 20.045 | -11.903 | 9.905 | 1.00 | 24.18 |
| ATOM | 2638 | CD2 | LEU | 1754 | 21.932 | -13.168 | 11.063 | 1.00 | 25.69 |
| ATOM | 2639 | C | LEU | 1754 | 19.860 | -16.870 | 10.763 | 1.00 | 28.74 |
| ATOM | 2640 | O | LEU | 1754 | 20.270 | -17.290 | 11.832 | 1.00 | 29.08 |
| ATOM | 2641 | N | ASP | 1755 | 18.834 | -17.419 | 10.130 | 1.00 | 29.97 |
| ATOM | 2643 | CA | ASP | 1755 | 18.109 | -18.519 | 10.732 | 1.00 | 31.58 |
| ATOM | 2644 | CB | ASP | 1755 | 16.944 | -18.930 | 9.843 | 1.00 | 36.47 |
| ATOM | 2645 | CG | ASP | 1755 | 16.100 | -20.005 | 10.467 | 1.00 | 39.40 |
| ATOM | 2646 | OD1 | ASP | 1755 | 15.731 | -19.869 | 11.651 | 1.00 | 45.91 |
| ATOM | 2647 | OD2 | ASP | 1755 | 15.813 | -20.995 | 9.774 | 1.00 | 45.68 |
| ATOM | 2648 | C | ASP | 1755 | 19.040 | -19.703 | 10.952 | 1.00 | 32.29 |
| ATOM | 2649 | O | ASP | 1755 | 18.978 | -20.380 | 11.979 | 1.00 | 31.66 |
| ATOM | 2650 | N | ARG | 1756 | 19.926 | -19.923 | 9.989 | 1.00 | 32.32 |
| ATOM | 2652 | CA | ARG | 1756 | 20.884 | -21.015 | 10.059 | 1.00 | 32.73 |
| ATOM | 2653 | CB | ARG | 1756 | 21.598 | -21.145 | 8.704 | 1.00 | 34.47 |
| ATOM | 2654 | CG | ARG | 1756 | 22.733 | -22.157 | 8.645 | 1.00 | 37.78 |
| ATOM | 2655 | CD | ARG | 1756 | 23.299 | -22.274 | 7.237 | 1.00 | 43.87 |
| ATOM | 2656 | NE | ARG | 1756 | 23.791 | -20.999 | 6.702 | 1.00 | 48.78 |
| ATOM | 2658 | CZ | ARG | 1756 | 24.890 | -20.380 | 7.122 | 1.00 | 52.92 |
| ATOM | 2659 | NH1 | ARG | 1756 | 25.630 | -20.914 | 8.091 | 1.00 | 55.88 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2662 | NH2 | ARG | 1756 | 25.237 | -19.214 | 6.593 | 1.00 | 52.53 |
| ATOM | 2665 | C | ARG | 1756 | 21.889 | -20.761 | 11.186 | 1.00 | 33.76 |
| ATOM | 2666 | O | ARG | 1756 | 22.131 | -21.619 | 12.049 | 1.00 | 34.53 |
| ATOM | 2667 | N | ILE | 1757 | 22.432 | -19.553 | 11.204 | 1.00 | 33.49 |
| ATOM | 2669 | CA | ILE | 1757 | 23.405 | -19.176 | 12.205 | 1.00 | 32.71 |
| ATOM | 2670 | CB | ILE | 1757 | 23.980 | -17.764 | 11.919 | 1.00 | 31.86 |
| ATOM | 2671 | CG2 | ILE | 1757 | 25.111 | -17.454 | 12.869 | 1.00 | 31.71 |
| ATOM | 2672 | CG1 | ILE | 1757 | 24.520 | -17.704 | 10.488 | 1.00 | 31.41 |
| ATOM | 2673 | CD1 | ILE | 1757 | 25.075 | -16.366 | 10.096 | 1.00 | 27.68 |
| ATOM | 2674 | C | ILE | 1757 | 22.807 | -19.236 | 13.604 | 1.00 | 34.20 |
| ATOM | 2675 | O | ILE | 1757 | 23.399 | -19.833 | 14.495 | 1.00 | 35.83 |
| ATOM | 2676 | N | VAL | 1758 | 21.620 | -18.667 | 13.792 | 1.00 | 35.40 |
| ATOM | 2678 | CA | VAL | 1758 | 20.981 | -18.653 | 15.108 | 1.00 | 37.49 |
| ATOM | 2679 | CB | VAL | 1758 | 19.501 | -18.160 | 15.061 | 1.00 | 34.42 |
| ATOM | 2680 | CG1 | VAL | 1758 | 18.899 | -18.199 | 16.456 | 1.00 | 37.37 |
| ATOM | 2681 | CG2 | VAL | 1758 | 19.403 | -16.742 | 14.519 | 1.00 | 30.02 |
| ATOM | 2682 | C | VAL | 1758 | 21.010 | -20.050 | 15.715 | 1.00 | 41.64 |
| ATOM | 2683 | O | VAL | 1758 | 21.533 | -20.246 | 16.817 | 1.00 | 43.69 |
| ATOM | 2684 | N | ALA | 1759 | 20.492 | -21.015 | 14.961 | 1.00 | 44.52 |
| ATOM | 2686 | CA | ALA | 1759 | 20.434 | -22.415 | 15.387 | 1.00 | 45.20 |
| ATOM | 2687 | CB | ALA | 1759 | 19.833 | -23.268 | 14.277 | 1.00 | 43.44 |
| ATOM | 2688 | C | ALA | 1759 | 21.791 | -22.968 | 15.795 | 1.00 | 45.91 |
| ATOM | 2689 | O | ALA | 1759 | 21.890 | -23.780 | 16.710 | 1.00 | 47.41 |
| ATOM | 2690 | N | LEU | 1760 | 22.833 | -22.511 | 15.120 | 1.00 | 47.70 |
| ATOM | 2692 | CA | LEU | 1760 | 24.190 | -22.960 | 15.399 | 1.00 | 50.91 |
| ATOM | 2693 | CB | LEU | 1760 | 25.015 | -22.912 | 14.109 | 1.00 | 52.93 |
| ATOM | 2694 | CG | LEU | 1760 | 24.448 | -23.723 | 12.947 | 1.00 | 57.55 |
| ATOM | 2695 | CD1 | LEU | 1760 | 25.189 | -23.390 | 11.660 | 1.00 | 60.76 |
| ATOM | 2696 | CD2 | LEU | 1760 | 24.539 | -25.208 | 13.273 | 1.00 | 58.66 |
| ATOM | 2697 | C | LEU | 1760 | 24.882 | -22.111 | 16.472 | 1.00 | 52.07 |
| ATOM | 2698 | O | LEU | 1760 | 25.967 | -22.459 | 16.953 | 1.00 | 51.95 |
| ATOM | 2699 | N | THR | 1761 | 24.267 | -21.000 | 16.850 | 1.00 | 52.05 |
| ATOM | 2701 | CA | THR | 1761 | 24.868 | -20.131 | 17.836 | 1.00 | 53.28 |
| ATOM | 2702 | CB | THR | 1761 | 24.362 | -18.693 | 17.673 | 1.00 | 54.58 |
| ATOM | 2703 | OG1 | THR | 1761 | 24.633 | -18.259 | 16.339 | 1.00 | 53.68 |
| ATOM | 2705 | CG2 | THR | 1761 | 25.090 | -17.762 | 18.621 | 1.00 | 55.45 |
| ATOM | 2706 | C | THR | 1761 | 24.715 | -20.619 | 19.272 | 1.00 | 53.31 |
| ATOM | 2707 | O | THR | 1761 | 23.629 | -20.986 | 19.713 | 1.00 | 53.89 |
| ATOM | 2708 | N | SER | 1762 | 25.832 | -20.617 | 19.993 | 1.00 | 53.51 |
| ATOM | 2710 | CA | SER | 1762 | 25.876 | -21.045 | 21.383 | 1.00 | 53.15 |
| ATOM | 2711 | CB | SER | 1762 | 27.340 | -21.131 | 21.830 | 1.00 | 57.27 |
| ATOM | 2712 | OG | SER | 1762 | 27.492 | -21.872 | 23.028 | 1.00 | 61.22 |
| ATOM | 2714 | C | SER | 1762 | 25.110 | -20.048 | 22.257 | 1.00 | 49.15 |
| ATOM | 2715 | O | SER | 1762 | 25.229 | -18.831 | 22.071 | 1.00 | 46.61 |
| ATOM | 3466 | N | ALA | 461 | 79.636 | 26.047 | 14.493 | 1.00 | 61.05 |
| ATOM | 3468 | CA | ALA | 461 | 79.609 | 24.852 | 13.654 | 1.00 | 58.10 |
| ATOM | 3469 | CB | ALA | 461 | 78.335 | 24.024 | 13.935 | 1.00 | 60.39 |
| ATOM | 3470 | C | ALA | 461 | 79.694 | 25.239 | 12.179 | 1.00 | 54.65 |
| ATOM | 3471 | O | ALA | 461 | 79.653 | 24.382 | 11.297 | 1.00 | 54.05 |
| ATOM | 3472 | N | ALA | 462 | 79.867 | 26.537 | 11.935 | 1.00 | 51.68 |
| ATOM | 3474 | CA | ALA | 462 | 79.972 | 27.085 | 10.584 | 1.00 | 48.47 |
| ATOM | 3475 | CB | ALA | 462 | 80.099 | 28.619 | 10.633 | 1.00 | 46.99 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3476 | C | ALA | 462 | 81.123 | 26.489 | 9.766 | 1.00 | 44.86 |
| ATOM | 3477 | O | ALA | 462 | 80.918 | 26.097 | 8.625 | 1.00 | 43.40 |
| ATOM | 3478 | N | TYR | 463 | 82.329 | 26.447 | 10.335 | 1.00 | 42.23 |
| ATOM | 3480 | CA | TYR | 463 | 83.493 | 25.913 | 9.629 | 1.00 | 39.04 |
| ATOM | 3481 | CB | TYR | 463 | 84.642 | 26.921 | 9.620 | 1.00 | 39.01 |
| ATOM | 3482 | CG | TYR | 463 | 84.354 | 28.126 | 8.743 | 1.00 | 41.95 |
| ATOM | 3483 | CD1 | TYR | 463 | 84.073 | 29.373 | 9.308 | 1.00 | 42.40 |
| ATOM | 3484 | CE1 | TYR | 463 | 83.754 | 30.466 | 8.512 | 1.00 | 42.02 |
| ATOM | 3485 | CD2 | TYR | 463 | 84.311 | 28.009 | 7.345 | 1.00 | 40.70 |
| ATOM | 3486 | CE2 | TYR | 463 | 83.992 | 29.099 | 6.542 | 1.00 | 37.09 |
| ATOM | 3487 | CZ | TYR | 463 | 83.716 | 30.320 | 7.134 | 1.00 | 39.19 |
| ATOM | 3488 | OH | TYR | 463 | 83.401 | 31.406 | 6.360 | 1.00 | 40.66 |
| ATOM | 3490 | C | TYR | 463 | 84.011 | 24.554 | 10.050 | 1.00 | 37.78 |
| ATOM | 3491 | O | TYR | 463 | 84.627 | 23.863 | 9.237 | 1.00 | 38.35 |
| ATOM | 3492 | N | GLU | 464 | 83.746 | 24.143 | 11.285 | 1.00 | 37.67 |
| ATOM | 3494 | CA | GLU | 464 | 84.212 | 22.841 | 11.747 | 1.00 | 38.57 |
| ATOM | 3495 | CB | GLU | 464 | 85.707 | 22.890 | 12.024 | 1.00 | 41.44 |
| ATOM | 3496 | CG | GLU | 464 | 86.093 | 23.870 | 13.108 | 1.00 | 47.87 |
| ATOM | 3497 | CD | GLU | 464 | 87.583 | 24.135 | 13.169 | 1.00 | 53.44 |
| ATOM | 3498 | OE1 | GLU | 464 | 87.998 | 24.983 | 13.990 | 1.00 | 56.72 |
| ATOM | 3499 | OE2 | GLU | 464 | 88.344 | 23.513 | 12.397 | 1.00 | 54.85 |
| ATOM | 3500 | C | GLU | 464 | 83.504 | 22.393 | 13.001 | 1.00 | 38.15 |
| ATOM | 3501 | O | GLU | 464 | 83.291 | 23.187 | 13.905 | 1.00 | 39.59 |
| ATOM | 3502 | N | LEU | 465 | 83.121 | 21.124 | 13.051 | 1.00 | 37.13 |
| ATOM | 3504 | CA | LEU | 465 | 82.457 | 20.608 | 14.236 | 1.00 | 37.93 |
| ATOM | 3505 | CB | LEU | 465 | 81.502 | 19.456 | 13.894 | 1.00 | 33.43 |
| ATOM | 3506 | CG | LEU | 465 | 80.455 | 19.609 | 12.787 | 1.00 | 31.12 |
| ATOM | 3507 | CD1 | LEU | 465 | 79.415 | 18.500 | 12.944 | 1.00 | 24.85 |
| ATOM | 3508 | CD2 | LEU | 465 | 79.797 | 20.980 | 12.855 | 1.00 | 29.05 |
| ATOM | 3509 | C | LEU | 465 | 83.540 | 20.090 | 15.166 | 1.00 | 41.02 |
| ATOM | 3510 | O | LEU | 465 | 84.703 | 19.936 | 14.763 | 1.00 | 40.24 |
| ATOM | 3511 | N | PRO | 466 | 83.198 | 19.884 | 16.441 | 1.00 | 43.58 |
| ATOM | 3512 | CD | PRO | 466 | 81.974 | 20.359 | 17.115 | 1.00 | 45.33 |
| ATOM | 3513 | CA | PRO | 466 | 84.170 | 19.374 | 17.415 | 1.00 | 44.72 |
| ATOM | 3514 | CB | PRO | 466 | 83.433 | 19.505 | 18.743 | 1.00 | 46.18 |
| ATOM | 3515 | CG | PRO | 466 | 82.486 | 20.679 | 18.496 | 1.00 | 48.84 |
| ATOM | 3516 | C | PRO | 466 | 84.447 | 17.909 | 17.101 | 1.00 | 44.52 |
| ATOM | 3517 | O | PRO | 466 | 83.616 | 17.228 | 16.509 | 1.00 | 43.38 |
| ATOM | 3518 | N | GLU | 467 | 85.610 | 17.421 | 17.492 | 1.00 | 47.75 |
| ATOM | 3520 | CA | GLU | 467 | 85.932 | 16.035 | 17.218 | 1.00 | 51.03 |
| ATOM | 3521 | CB | GLU | 467 | 87.354 | 15.913 | 16.659 | 1.00 | 56.11 |
| ATOM | 3522 | CG | GLU | 467 | 87.615 | 14.557 | 16.000 | 1.00 | 62.27 |
| ATOM | 3523 | CD | GLU | 467 | 88.927 | 14.489 | 15.242 | 1.00 | 66.39 |
| ATOM | 3524 | OE1 | GLU | 467 | 89.688 | 15.490 | 15.243 | 1.00 | 69.85 |
| ATOM | 3525 | OE2 | GLU | 467 | 89.182 | 13.418 | 14.643 | 1.00 | 66.09 |
| ATOM | 3526 | C | GLU | 467 | 85.749 | 15.136 | 18.435 | 1.00 | 49.62 |
| ATOM | 3527 | O | GLU | 467 | 85.767 | 15.601 | 19.578 | 1.00 | 49.62 |
| ATOM | 3528 | N | ASP | 468 | 85.516 | 13.856 | 18.166 | 1.00 | 48.07 |
| ATOM | 3530 | CA | ASP | 468 | 85.352 | 12.843 | 19.198 | 1.00 | 46.32 |
| ATOM | 3531 | CB | ASP | 468 | 83.880 | 12.679 | 19.587 | 1.00 | 45.15 |
| ATOM | 3532 | CG | ASP | 468 | 83.678 | 11.740 | 20.779 | 1.00 | 44.19 |
| ATOM | 3533 | OD1 | ASP | 468 | 82.544 | 11.709 | 21.309 | 1.00 | 42.04 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3534 | OD2 | ASP | 468 | 84.629 | 11.033 | 21.188 | 1.00 | 38.14 |
| ATOM | 3535 | C | ASP | 468 | 85.877 | 11.556 | 18.580 | 1.00 | 45.54 |
| ATOM | 3536 | O | ASP | 468 | 85.141 | 10.815 | 17.928 | 1.00 | 45.94 |
| ATOM | 3537 | N | PRO | 469 | 87.181 | 11.308 | 18.732 | 1.00 | 45.89 |
| ATOM | 3538 | CD | PRO | 469 | 88.111 | 12.189 | 19.464 | 1.00 | 45.11 |
| ATOM | 3539 | CA | PRO | 469 | 87.885 | 10.130 | 18.215 | 1.00 | 45.91 |
| ATOM | 3540 | CB | PRO | 469 | 89.208 | 10.187 | 18.968 | 1.00 | 45.90 |
| ATOM | 3541 | CG | PRO | 469 | 89.456 | 11.662 | 19.042 | 1.00 | 45.73 |
| ATOM | 3542 | C | PRO | 469 | 87.170 | 8.806 | 18.473 | 1.00 | 45.48 |
| ATOM | 3543 | O | PRO | 469 | 87.188 | 7.905 | 17.629 | 1.00 | 46.83 |
| ATOM | 3544 | N | ARG | 470 | 86.495 | 8.717 | 19.613 | 1.00 | 42.12 |
| ATOM | 3546 | CA | ARG | 470 | 85.786 | 7.506 | 19.999 | 1.00 | 41.21 |
| ATOM | 3547 | CB | ARG | 470 | 85.083 | 7.704 | 21.331 | 1.00 | 43.14 |
| ATOM | 3548 | CG | ARG | 470 | 85.885 | 8.424 | 22.375 | 1.00 | 45.68 |
| ATOM | 3549 | CD | ARG | 470 | 85.014 | 8.705 | 23.564 | 1.00 | 45.98 |
| ATOM | 3550 | NE | ARG | 470 | 83.802 | 9.417 | 23.184 | 1.00 | 47.28 |
| ATOM | 3552 | CZ | ARG | 470 | 82.921 | 9.877 | 24.057 | 1.00 | 50.54 |
| ATOM | 3553 | NH1 | ARG | 470 | 83.127 | 9.687 | 25.354 | 1.00 | 47.56 |
| ATOM | 3556 | NH2 | ARG | 470 | 81.843 | 10.527 | 23.637 | 1.00 | 54.59 |
| ATOM | 3559 | C | ARG | 470 | 84.736 | 7.058 | 19.004 | 1.00 | 40.57 |
| ATOM | 3560 | O | ARG | 470 | 84.411 | 5.877 | 18.941 | 1.00 | 43.13 |
| ATOM | 3561 | N | TRP | 471 | 84.182 | 8.014 | 18.268 | 1.00 | 38.07 |
| ATOM | 3563 | CA | TRP | 471 | 83.124 | 7.736 | 17.314 | 1.00 | 35.09 |
| ATOM | 3564 | CB | TRP | 471 | 81.890 | 8.515 | 17.739 | 1.00 | 33.42 |
| ATOM | 3565 | CG | TRP | 471 | 81.259 | 7.958 | 18.952 | 1.00 | 31.71 |
| ATOM | 3566 | CD2 | TRP | 471 | 80.512 | 6.740 | 19.026 | 1.00 | 34.81 |
| ATOM | 3567 | CE2 | TRP | 471 | 80.061 | 6.610 | 20.355 | 1.00 | 33.17 |
| ATOM | 3568 | CE3 | TRP | 471 | 80.174 | 5.744 | 18.092 | 1.00 | 37.60 |
| ATOM | 3569 | CD1 | TRP | 471 | 81.246 | 8.503 | 20.199 | 1.00 | 25.70 |
| ATOM | 3570 | NE1 | TRP | 471 | 80.525 | 7.697 | 21.051 | 1.00 | 28.79 |
| ATOM | 3572 | CZ2 | TRP | 471 | 79.289 | 5.522 | 20.776 | 1.00 | 35.80 |
| ATOM | 3573 | CZ3 | TRP | 471 | 79.409 | 4.660 | 18.509 | 1.00 | 35.52 |
| ATOM | 3574 | CH2 | TRP | 471 | 78.973 | 4.560 | 19.839 | 1.00 | 34.51 |
| ATOM | 3575 | C | TRP | 471 | 83.432 | 8.065 | 15.872 | 1.00 | 35.77 |
| ATOM | 3576 | O | TRP | 471 | 82.690 | 7.670 | 14.968 | 1.00 | 37.45 |
| ATOM | 3577 | N | GLU | 472 | 84.533 | 8.770 | 15.651 | 1.00 | 34.76 |
| ATOM | 3579 | CA | GLU | 472 | 84.895 | 9.184 | 14.308 | 1.00 | 34.51 |
| ATOM | 3580 | CB | GLU | 472 | 86.065 | 10.174 | 14.365 | 1.00 | 32.30 |
| ATOM | 3581 | CG | GLU | 472 | 86.221 | 11.038 | 13.103 | 1.00 | 36.57 |
| ATOM | 3582 | CD | GLU | 472 | 85.082 | 12.035 | 12.872 | 1.00 | 36.34 |
| ATOM | 3583 | OE1 | GLU | 472 | 84.515 | 12.558 | 13.857 | 1.00 | 36.01 |
| ATOM | 3584 | OE2 | GLU | 472 | 84.777 | 12.318 | 11.694 | 1.00 | 31.95 |
| ATOM | 3585 | C | GLU | 472 | 85.219 | 8.034 | 13.364 | 1.00 | 33.90 |
| ATOM | 3586 | O | GLU | 472 | 85.896 | 7.082 | 13.745 | 1.00 | 33.77 |
| ATOM | 3587 | N | LEU | 473 | 84.667 | 8.094 | 12.158 | 1.00 | 33.58 |
| ATOM | 3589 | CA | LEU | 473 | 84.944 | 7.095 | 11.146 | 1.00 | 34.82 |
| ATOM | 3590 | CB | LEU | 473 | 83.714 | 6.234 | 10.847 | 1.00 | 32.59 |
| ATOM | 3591 | CG | LEU | 473 | 84.020 | 5.091 | 9.867 | 1.00 | 33.78 |
| ATOM | 3592 | CD1 | LEU | 473 | 84.786 | 4.000 | 10.578 | 1.00 | 32.94 |
| ATOM | 3593 | CD2 | LEU | 473 | 82.759 | 4.518 | 9.273 | 1.00 | 35.34 |
| ATOM | 3594 | C | LEU | 473 | 85.380 | 7.828 | 9.883 | 1.00 | 37.95 |
| ATOM | 3595 | O | LEU | 473 | 84.720 | 8.781 | 9.457 | 1.00 | 39.55 |

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|---|---|---|---|---|---|---|---|---|
| ATOM | 3596 | N | PRO | 474 | 86.522 | 7.423 | 9.299 | 1.00 38.99 |
| ATOM | 3597 | CD | PRO | 474 | 87.455 | 6.453 | 9.899 | 1.00 38.76 |
| ATOM | 3598 | CA | PRO | 474 | 87.094 | 8.004 | 8.080 | 1.00 39.37 |
| ATOM | 3599 | CB | PRO | 474 | 88.382 | 7.201 | 7.906 | 1.00 40.18 |
| ATOM | 3600 | CG | PRO | 474 | 88.767 | 6.883 | 9.310 | 1.00 37.76 |
| ATOM | 3601 | C | PRO | 474 | 86.165 | 7.794 | 6.890 | 1.00 40.94 |
| ATOM | 3602 | O | PRO | 474 | 85.865 | 6.653 | 6.532 | 1.00 43.98 |
| ATOM | 3603 | N | ARG | 475 | 85.762 | 8.886 | 6.245 | 1.00 40.66 |
| ATOM | 3605 | CA | ARG | 475 | 84.850 | 8.840 | 5.101 | 1.00 40.66 |
| ATOM | 3606 | CB | ARG | 475 | 84.776 | 10.216 | 4.448 | 1.00 37.94 |
| ATOM | 3607 | CG | ARG | 475 | 84.354 | 11.300 | 5.415 | 1.00 36.12 |
| ATOM | 3608 | CD | ARG | 475 | 84.340 | 12.697 | 4.800 | 1.00 35.92 |
| ATOM | 3609 | NE | ARG | 475 | 83.932 | 13.677 | 5.801 | 1.00 30.14 |
| ATOM | 3611 | CZ | ARG | 475 | 82.671 | 13.878 | 6.170 | 1.00 28.45 |
| ATOM | 3612 | NH1 | ARG | 475 | 81.688 | 13.197 | 5.599 | 1.00 28.41 |
| ATOM | 3615 | NH2 | ARG | 475 | 82.410 | 14.666 | 7.197 | 1.00 27.85 |
| ATOM | 3618 | C | ARG | 475 | 85.141 | 7.766 | 4.046 | 1.00 41.44 |
| ATOM | 3619 | O | ARG | 475 | 84.223 | 7.189 | 3.470 | 1.00 41.40 |
| ATOM | 3620 | N | ASP | 476 | 86.419 | 7.475 | 3.830 | 1.00 44.99 |
| ATOM | 3622 | CA | ASP | 476 | 86.836 | 6.477 | 2.849 | 1.00 50.62 |
| ATOM | 3623 | CB | ASP | 476 | 88.344 | 6.540 | 2.644 | 1.00 54.47 |
| ATOM | 3624 | CG | ASP | 476 | 89.105 | 5.969 | 3.819 | 1.00 60.03 |
| ATOM | 3625 | OD1 | ASP | 476 | 89.569 | 4.810 | 3.722 | 1.00 65.09 |
| ATOM | 3626 | OD2 | ASP | 476 | 89.216 | 6.669 | 4.846 | 1.00 62.62 |
| ATOM | 3627 | C | ASP | 476 | 86.436 | 5.054 | 3.263 | 1.00 51.16 |
| ATOM | 3628 | O | ASP | 476 | 86.678 | 4.091 | 2.530 | 1.00 53.06 |
| ATOM | 3629 | N | ARG | 477 | 85.900 | 4.916 | 4.471 | 1.00 49.58 |
| ATOM | 3631 | CA | ARG | 477 | 85.443 | 3.623 | 4.968 | 1.00 47.34 |
| ATOM | 3632 | CB | ARG | 477 | 86.040 | 3.359 | 6.341 | 1.00 48.85 |
| ATOM | 3633 | CG | ARG | 477 | 87.481 | 2.924 | 6.265 | 1.00 52.11 |
| ATOM | 3634 | CD | ARG | 477 | 88.169 | 3.079 | 7.591 | 1.00 53.63 |
| ATOM | 3635 | NE | ARG | 477 | 87.515 | 2.345 | 8.665 | 1.00 54.86 |
| ATOM | 3637 | CZ | ARG | 477 | 87.932 | 2.363 | 9.927 | 1.00 57.15 |
| ATOM | 3638 | NH1 | ARG | 477 | 89.000 | 3.076 | 10.264 | 1.00 55.98 |
| ATOM | 3641 | NH2 | ARG | 477 | 87.269 | 1.691 | 10.855 | 1.00 58.31 |
| ATOM | 3644 | C | ARG | 477 | 83.915 | 3.563 | 5.020 | 1.00 44.70 |
| ATOM | 3645 | O | ARG | 477 | 83.339 | 2.780 | 5.770 | 1.00 44.63 |
| ATOM | 3646 | N | LEU | 478 | 83.274 | 4.366 | 4.179 | 1.00 41.95 |
| ATOM | 3648 | CA | LEU | 478 | 81.832 | 4.440 | 4.118 | 1.00 38.58 |
| ATOM | 3649 | CB | LEU | 478 | 81.374 | 5.609 | 4.980 | 1.00 33.17 |
| ATOM | 3650 | CG | LEU | 478 | 79.872 | 5.731 | 5.183 | 1.00 29.07 |
| ATOM | 3651 | CD1 | LEU | 478 | 79.393 | 4.592 | 6.052 | 1.00 28.25 |
| ATOM | 3652 | CD2 | LEU | 478 | 79.590 | 7.059 | 5.836 | 1.00 30.79 |
| ATOM | 3653 | C | LEU | 478 | 81.432 | 4.710 | 2.674 | 1.00 38.93 |
| ATOM | 3654 | O | LEU | 478 | 81.938 | 5.647 | 2.071 | 1.00 41.75 |
| ATOM | 3655 | N | VAL | 479 | 80.562 | 3.880 | 2.107 | 1.00 37.96 |
| ATOM | 3657 | CA | VAL | 479 | 80.113 | 4.086 | 0.730 | 1.00 37.87 |
| ATOM | 3658 | CB | VAL | 479 | 80.468 | 2.882 | -0.192 | 1.00 36.47 |
| ATOM | 3659 | CG1 | VAL | 479 | 80.001 | 3.145 | -1.612 | 1.00 34.43 |
| ATOM | 3660 | CG2 | VAL | 479 | 81.972 | 2.651 | -0.187 | 1.00 34.33 |
| ATOM | 3661 | C | VAL | 479 | 78.609 | 4.299 | 0.775 | 1.00 38.10 |
| ATOM | 3662 | O | VAL | 479 | 77.846 | 3.366 | 1.019 | 1.00 40.13 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3663 | N | LEU | 480 | 78.184 | 5.537 | 0.552 | 1.00 | 38.05 |
| ATOM | 3665 | CA | LEU | 480 | 76.766 | 5.879 | 0.606 | 1.00 | 35.90 |
| ATOM | 3666 | CB | LEU | 480 | 76.568 | 7.393 | 0.475 | 1.00 | 33.98 |
| ATOM | 3667 | CG | LEU | 480 | 77.276 | 8.257 | 1.536 | 1.00 | 32.84 |
| ATOM | 3668 | CD1 | LEU | 480 | 77.003 | 9.749 | 1.273 | 1.00 | 29.68 |
| ATOM | 3669 | CD2 | LEU | 480 | 76.828 | 7.861 | 2.943 | 1.00 | 26.03 |
| ATOM | 3670 | C | LEU | 480 | 76.015 | 5.146 | -0.476 | 1.00 | 34.99 |
| ATOM | 3671 | O | LEU | 480 | 76.573 | 4.864 | -1.526 | 1.00 | 36.12 |
| ATOM | 3672 | N | GLY | 481 | 74.753 | 4.836 | -0.223 | 1.00 | 35.21 |
| ATOM | 3674 | CA | GLY | 481 | 73.965 | 4.120 | -1.204 | 1.00 | 34.79 |
| ATOM | 3675 | C | GLY | 481 | 72.544 | 4.608 | -1.332 | 1.00 | 36.31 |
| ATOM | 3676 | O | GLY | 481 | 72.237 | 5.775 | -1.046 | 1.00 | 38.30 |
| ATOM | 3677 | N | LYS | 482 | 71.665 | 3.705 | -1.761 | 1.00 | 35.59 |
| ATOM | 3679 | CA | LYS | 482 | 70.257 | 4.007 | -1.959 | 1.00 | 35.24 |
| ATOM | 3680 | CB | LYS | 482 | 69.488 | 2.698 | -2.207 | 1.00 | 35.69 |
| ATOM | 3681 | C | LYS | 482 | 69.585 | 4.763 | -0.823 | 1.00 | 36.31 |
| ATOM | 3682 | O | LYS | 482 | 69.752 | 4.421 | 0.352 | 1.00 | 34.90 |
| ATOM | 3683 | N | PRO | 483 | 68.787 | 5.786 | -1.157 | 1.00 | 38.08 |
| ATOM | 3684 | CD | PRO | 483 | 68.432 | 6.320 | -2.483 | 1.00 | 39.57 |
| ATOM | 3685 | CA | PRO | 483 | 68.097 | 6.566 | -0.135 | 1.00 | 41.08 |
| ATOM | 3686 | CB | PRO | 483 | 67.300 | 7.560 | -0.987 | 1.00 | 39.80 |
| ATOM | 3687 | CG | PRO | 483 | 68.268 | 7.819 | -2.157 | 1.00 | 37.87 |
| ATOM | 3688 | C | PRO | 483 | 67.130 | 5.652 | 0.606 | 1.00 | 42.11 |
| ATOM | 3689 | O | PRO | 483 | 66.306 | 4.994 | -0.025 | 1.00 | 43.01 |
| ATOM | 3690 | N | LEU | 484 | 67.199 | 5.624 | 1.937 | 1.00 | 41.06 |
| ATOM | 3692 | CA | LEU | 484 | 66.293 | 4.823 | 2.751 | 1.00 | 38.47 |
| ATOM | 3693 | CB | LEU | 484 | 67.040 | 4.307 | 3.990 | 1.00 | 32.45 |
| ATOM | 3694 | CG | LEU | 484 | 67.968 | 3.098 | 3.809 | 1.00 | 27.68 |
| ATOM | 3695 | CD1 | LEU | 484 | 68.569 | 2.710 | 5.147 | 1.00 | 20.29 |
| ATOM | 3696 | CD2 | LEU | 484 | 67.181 | 1.964 | 3.225 | 1.00 | 23.20 |
| ATOM | 3697 | C | LEU | 484 | 65.084 | 5.637 | 3.180 | 1.00 | 42.18 |
| ATOM | 3698 | O | LEU | 484 | 65.227 | 6.699 | 3.814 | 1.00 | 44.50 |
| ATOM | 3699 | N | GLY | 485 | 63.893 | 5.170 | 2.817 | 1.00 | 45.68 |
| ATOM | 3701 | CA | GLY | 485 | 62.692 | 5.863 | 3.220 | 1.00 | 49.88 |
| ATOM | 3702 | C | GLY | 485 | 62.216 | 7.008 | 2.337 | 1.00 | 53.01 |
| ATOM | 3703 | O | GLY | 485 | 62.438 | 7.005 | 1.117 | 1.00 | 50.26 |
| ATOM | 3704 | N | GLU | 486 | 61.592 | 8.020 | 2.949 | 1.00 | 56.24 |
| ATOM | 3706 | CA | GLU | 486 | 61.064 | 9.183 | 2.257 | 1.00 | 58.07 |
| ATOM | 3707 | CB | GLU | 486 | 59.666 | 8.845 | 1.682 | 1.00 | 55.60 |
| ATOM | 3708 | C | GLU | 486 | 60.995 | 10.477 | 3.088 | 1.00 | 59.35 |
| ATOM | 3709 | O | GLU | 486 | 60.019 | 11.226 | 3.000 | 1.00 | 61.44 |
| ATOM | 3710 | N | GLY | 487 | 62.027 | 10.747 | 3.879 | 1.00 | 59.60 |
| ATOM | 3712 | CA | GLY | 487 | 62.066 | 11.964 | 4.652 | 1.00 | 59.75 |
| ATOM | 3713 | C | GLY | 487 | 61.337 | 11.959 | 5.974 | 1.00 | 61.44 |
| ATOM | 3714 | O | GLY | 487 | 61.231 | 12.979 | 6.627 | 1.00 | 61.96 |
| ATOM | 3715 | N | ALA | 488 | 60.820 | 10.800 | 6.377 | 1.00 | 59.69 |
| ATOM | 3717 | CA | ALA | 488 | 60.134 | 10.709 | 7.657 | 1.00 | 57.27 |
| ATOM | 3718 | CB | ALA | 488 | 59.489 | 9.337 | 7.825 | 1.00 | 58.05 |
| ATOM | 3719 | C | ALA | 488 | 61.137 | 10.970 | 8.754 | 1.00 | 56.28 |
| ATOM | 3720 | O | ALA | 488 | 60.810 | 11.446 | 9.834 | 1.00 | 57.31 |
| ATOM | 3721 | N | PHE | 489 | 62.389 | 10.630 | 8.480 | 1.00 | 54.40 |
| ATOM | 3723 | CA | PHE | 489 | 63.462 | 10.830 | 9.466 | 1.00 | 54.56 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3724 | CB | PHE | 489 | 64.161 | 9.500 | 9.770 | 1.00 | 49.88 |
| ATOM | 3725 | CG | PHE | 489 | 63.222 | 8.454 | 10.352 | 1.00 | 45.21 |
| ATOM | 3726 | CD1 | PHE | 489 | 62.505 | 7.585 | 9.516 | 1.00 | 43.48 |
| ATOM | 3727 | CD2 | PHE | 489 | 63.017 | 8.344 | 11.738 | 1.00 | 40.99 |
| ATOM | 3728 | CE1 | PHE | 489 | 61.625 | 6.653 | 10.039 | 1.00 | 36.69 |
| ATOM | 3729 | CE2 | PHE | 489 | 62.138 | 7.411 | 12.257 | 1.00 | 35.02 |
| ATOM | 3730 | CZ | PHE | 489 | 61.433 | 6.558 | 11.407 | 1.00 | 34.73 |
| ATOM | 3731 | C | PHE | 489 | 64.456 | 11.896 | 8.974 | 1.00 | 56.31 |
| ATOM | 3732 | O | PHE | 489 | 65.372 | 12.276 | 9.692 | 1.00 | 59.05 |
| ATOM | 3733 | N | GLY | 490 | 64.285 | 12.375 | 7.735 | 1.00 | 56.56 |
| ATOM | 3735 | CA | GLY | 490 | 65.141 | 13.400 | 7.143 | 1.00 | 55.60 |
| ATOM | 3736 | C | GLY | 490 | 65.899 | 12.778 | 5.993 | 1.00 | 54.79 |
| ATOM | 3737 | O | GLY | 490 | 65.357 | 11.854 | 5.366 | 1.00 | 57.10 |
| ATOM | 3738 | N | GLN | 491 | 67.073 | 13.304 | 5.634 | 1.00 | 53.44 |
| ATOM | 3740 | CA | GLN | 491 | 67.829 | 12.658 | 4.562 | 1.00 | 52.60 |
| ATOM | 3741 | CB | GLN | 491 | 68.760 | 13.580 | 3.777 | 1.00 | 53.48 |
| ATOM | 3742 | CG | GLN | 491 | 69.422 | 12.818 | 2.629 | 1.00 | 57.19 |
| ATOM | 3743 | CD | GLN | 491 | 70.046 | 13.696 | 1.548 | 1.00 | 62.09 |
| ATOM | 3744 | OE1 | GLN | 491 | 70.113 | 14.893 | 1.701 | 1.00 | 70.26 |
| ATOM | 3745 | NE2 | GLN | 491 | 70.453 | 13.082 | 0.441 | 1.00 | 62.78 |
| ATOM | 3748 | C | GLN | 491 | 68.632 | 11.518 | 5.165 | 1.00 | 49.89 |
| ATOM | 3749 | O | GLN | 491 | 69.669 | 11.704 | 5.805 | 1.00 | 49.56 |
| ATOM | 3750 | N | VAL | 492 | 68.103 | 10.318 | 4.984 | 1.00 | 47.83 |
| ATOM | 3752 | CA | VAL | 492 | 68.705 | 9.093 | 5.456 | 1.00 | 46.38 |
| ATOM | 3753 | CB | VAL | 492 | 67.760 | 8.320 | 6.412 | 1.00 | 45.61 |
| ATOM | 3754 | CG1 | VAL | 492 | 68.412 | 7.045 | 6.932 | 1.00 | 46.70 |
| ATOM | 3755 | CG2 | VAL | 492 | 67.361 | 9.211 | 7.606 | 1.00 | 46.97 |
| ATOM | 3756 | C | VAL | 492 | 69.004 | 8.200 | 4.253 | 1.00 | 45.23 |
| ATOM | 3757 | O | VAL | 492 | 68.181 | 8.044 | 3.349 | 1.00 | 45.17 |
| ATOM | 3758 | N | VAL | 493 | 70.210 | 7.654 | 4.208 | 1.00 | 43.75 |
| ATOM | 3760 | CA | VAL | 493 | 70.599 | 6.780 | 3.109 | 1.00 | 44.71 |
| ATOM | 3761 | CB | VAL | 493 | 71.608 | 7.471 | 2.148 | 1.00 | 46.20 |
| ATOM | 3762 | CG1 | VAL | 493 | 71.159 | 8.902 | 1.838 | 1.00 | 46.16 |
| ATOM | 3763 | CG2 | VAL | 493 | 73.045 | 7.428 | 2.706 | 1.00 | 42.06 |
| ATOM | 3764 | C | VAL | 493 | 71.205 | 5.482 | 3.624 | 1.00 | 44.09 |
| ATOM | 3765 | O | VAL | 493 | 71.701 | 5.402 | 4.745 | 1.00 | 43.73 |
| ATOM | 3766 | N | LEU | 494 | 71.102 | 4.448 | 2.809 | 1.00 | 43.38 |
| ATOM | 3768 | CA | LEU | 494 | 71.682 | 3.158 | 3.142 | 1.00 | 43.29 |
| ATOM | 3769 | CB | LEU | 494 | 70.988 | 2.030 | 2.366 | 1.00 | 43.38 |
| ATOM | 3770 | CG | LEU | 494 | 71.563 | 0.614 | 2.431 | 1.00 | 39.77 |
| ATOM | 3771 | CD1 | LEU | 494 | 71.809 | 0.201 | 3.850 | 1.00 | 36.38 |
| ATOM | 3772 | CD2 | LEU | 494 | 70.600 | -0.337 | 1.760 | 1.00 | 42.50 |
| ATOM | 3773 | C | LEU | 494 | 73.139 | 3.280 | 2.725 | 1.00 | 42.72 |
| ATOM | 3774 | O | LEU | 494 | 73.435 | 3.929 | 1.720 | 1.00 | 43.83 |
| ATOM | 3775 | N | ALA | 495 | 74.044 | 2.698 | 3.499 | 1.00 | 40.80 |
| ATOM | 3777 | CA | ALA | 495 | 75.456 | 2.785 | 3.183 | 1.00 | 43.80 |
| ATOM | 3778 | CB | ALA | 495 | 76.059 | 4.032 | 3.821 | 1.00 | 43.76 |
| ATOM | 3779 | C | ALA | 495 | 76.171 | 1.546 | 3.682 | 1.00 | 46.68 |
| ATOM | 3780 | O | ALA | 495 | 75.668 | 0.838 | 4.551 | 1.00 | 48.52 |
| ATOM | 3781 | N | GLU | 496 | 77.330 | 1.258 | 3.104 | 1.00 | 49.13 |
| ATOM | 3783 | CA | GLU | 496 | 78.112 | 0.103 | 3.519 | 1.00 | 49.79 |
| ATOM | 3784 | CB | GLU | 496 | 78.524 | -0.732 | 2.318 | 1.00 | 53.83 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3785 | CG | GLU | 496 | 77.350 | -1.224 | 1.496 | 1.00 | 61.33 |
| ATOM | 3786 | CD | GLU | 496 | 77.623 | -2.561 | 0.862 | 1.00 | 64.74 |
| ATOM | 3787 | OE1 | GLU | 496 | 76.704 | -3.411 | 0.883 | 1.00 | 70.08 |
| ATOM | 3788 | OE2 | GLU | 496 | 78.751 | -2.760 | 0.356 | 1.00 | 64.12 |
| ATOM | 3789 | C | GLU | 496 | 79.333 | 0.601 | 4.230 | 1.00 | 48.46 |
| ATOM | 3790 | O | GLU | 496 | 80.192 | 1.236 | 3.631 | 1.00 | 48.79 |
| ATOM | 3791 | N | ALA | 497 | 79.373 | 0.375 | 5.530 | 1.00 | 49.25 |
| ATOM | 3793 | CA | ALA | 497 | 80.503 | 0.810 | 6.334 | 1.00 | 49.99 |
| ATOM | 3794 | CB | ALA | 497 | 80.048 | 1.156 | 7.732 | 1.00 | 48.16 |
| ATOM | 3795 | C | ALA | 497 | 81.544 | -0.301 | 6.373 | 1.00 | 51.53 |
| ATOM | 3796 | O | ALA | 497 | 81.191 | -1.473 | 6.409 | 1.00 | 52.41 |
| ATOM | 3797 | N | ILE | 498 | 82.821 | 0.061 | 6.335 | 1.00 | 52.35 |
| ATOM | 3799 | CA | ILE | 498 | 83.892 | -0.928 | 6.369 | 1.00 | 52.03 |
| ATOM | 3800 | CB | ILE | 498 | 84.843 | -0.797 | 5.145 | 1.00 | 52.83 |
| ATOM | 3801 | CG2 | ILE | 498 | 85.990 | -1.795 | 5.253 | 1.00 | 51.43 |
| ATOM | 3802 | CG1 | ILE | 498 | 84.077 | -1.006 | 3.830 | 1.00 | 53.85 |
| ATOM | 3803 | CD1 | ILE | 498 | 83.411 | 0.254 | 3.271 | 1.00 | 55.62 |
| ATOM | 3804 | C | ILE | 498 | 84.702 | -0.802 | 7.654 | 1.00 | 52.74 |
| ATOM | 3805 | O | ILE | 498 | 85.133 | 0.293 | 8.026 | 1.00 | 52.14 |
| ATOM | 3806 | N | GLY | 499 | 84.835 | -1.926 | 8.354 | 1.00 | 52.58 |
| ATOM | 3808 | CA | GLY | 499 | 85.600 | -1.974 | 9.592 | 1.00 | 53.03 |
| ATOM | 3809 | C | GLY | 499 | 85.165 | -1.113 | 10.771 | 1.00 | 53.67 |
| ATOM | 3810 | O | GLY | 499 | 86.012 | -0.544 | 11.463 | 1.00 | 53.99 |
| ATOM | 3811 | N | LEU | 500 | 83.862 | -1.045 | 11.034 | 1.00 | 53.60 |
| ATOM | 3813 | CA | LEU | 500 | 83.337 | -0.245 | 12.141 | 1.00 | 51.00 |
| ATOM | 3814 | CB | LEU | 500 | 81.841 | -0.499 | 12.317 | 1.00 | 49.38 |
| ATOM | 3815 | CG | LEU | 500 | 80.901 | -0.024 | 11.212 | 1.00 | 47.62 |
| ATOM | 3816 | CD1 | LEU | 500 | 79.483 | -0.454 | 11.543 | 1.00 | 47.25 |
| ATOM | 3817 | CD2 | LEU | 500 | 80.992 | 1.486 | 11.081 | 1.00 | 47.38 |
| ATOM | 3818 | C | LEU | 500 | 84.060 | -0.573 | 13.433 | 1.00 | 51.09 |
| ATOM | 3819 | O | LEU | 500 | 84.396 | -1.734 | 13.670 | 1.00 | 53.76 |
| ATOM | 3820 | N | PRO | 505 | 87.588 | -5.968 | 10.545 | 1.00 | 81.81 |
| ATOM | 3821 | CD | PRO | 505 | 88.588 | -6.677 | 11.357 | 1.00 | 81.96 |
| ATOM | 3822 | CA | PRO | 505 | 88.105 | -4.664 | 10.109 | 1.00 | 80.56 |
| ATOM | 3823 | CB | PRO | 505 | 89.501 | -4.622 | 10.735 | 1.00 | 80.75 |
| ATOM | 3824 | CG | PRO | 505 | 89.868 | -6.070 | 10.860 | 1.00 | 82.32 |
| ATOM | 3825 | C | PRO | 505 | 88.139 | -4.477 | 8.588 | 1.00 | 78.53 |
| ATOM | 3826 | O | PRO | 505 | 88.462 | -3.400 | 8.085 | 1.00 | 77.85 |
| ATOM | 3827 | N | ASN | 506 | 87.792 | -5.532 | 7.865 | 1.00 | 77.09 |
| ATOM | 3829 | CA | ASN | 506 | 87.747 | -5.484 | 6.411 | 1.00 | 75.57 |
| ATOM | 3830 | CB | ASN | 506 | 88.799 | -6.415 | 5.806 | 1.00 | 75.80 |
| ATOM | 3831 | C | ASN | 506 | 86.347 | -5.929 | 6.008 | 1.00 | 74.33 |
| ATOM | 3832 | O | ASN | 506 | 86.044 | -6.117 | 4.826 | 1.00 | 73.76 |
| ATOM | 3833 | N | ARG | 507 | 85.496 | -6.092 | 7.018 | 1.00 | 71.72 |
| ATOM | 3835 | CA | ARG | 507 | 84.120 | -6.509 | 6.820 | 1.00 | 69.28 |
| ATOM | 3836 | CB | ARG | 507 | 83.619 | -7.257 | 8.054 | 1.00 | 70.64 |
| ATOM | 3837 | C | ARG | 507 | 83.258 | -5.284 | 6.605 | 1.00 | 65.87 |
| ATOM | 3838 | O | ARG | 507 | 83.445 | -4.262 | 7.274 | 1.00 | 65.40 |
| ATOM | 3839 | N | VAL | 508 | 82.363 | -5.358 | 5.628 | 1.00 | 62.01 |
| ATOM | 3841 | CA | VAL | 508 | 81.464 | -4.248 | 5.381 | 1.00 | 58.41 |
| ATOM | 3842 | CB | VAL | 508 | 81.043 | -4.136 | 3.915 | 1.00 | 57.18 |
| ATOM | 3843 | CG1 | VAL | 508 | 82.251 | -3.893 | 3.046 | 1.00 | 61.04 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3844 | CG2 | VAL | 508 | 80.310 | -5.383 | 3.466 | 1.00 | 60.74 |
| ATOM | 3845 | C | VAL | 508 | 80.257 | -4.552 | 6.246 | 1.00 | 56.61 |
| ATOM | 3846 | O | VAL | 508 | 79.964 | -5.716 | 6.529 | 1.00 | 55.82 |
| ATOM | 3847 | N | THR | 509 | 79.572 | -3.501 | 6.665 | 1.00 | 54.85 |
| ATOM | 3849 | CA | THR | 509 | 78.396 | -3.610 | 7.501 | 1.00 | 49.28 |
| ATOM | 3850 | CB | THR | 509 | 78.705 | -3.144 | 8.934 | 1.00 | 47.98 |
| ATOM | 3851 | OG1 | THR | 509 | 79.938 | -3.727 | 9.356 | 1.00 | 43.39 |
| ATOM | 3853 | CG2 | THR | 509 | 77.606 | -3.565 | 9.903 | 1.00 | 47.57 |
| ATOM | 3854 | C | THR | 509 | 77.381 | -2.674 | 6.865 | 1.00 | 46.71 |
| ATOM | 3855 | O | THR | 509 | 77.675 | -1.507 | 6.625 | 1.00 | 48.59 |
| ATOM | 3856 | N | LYS | 510 | 76.238 | -3.208 | 6.470 | 1.00 | 44.75 |
| ATOM | 3858 | CA | LYS | 510 | 75.202 | -2.372 | 5.889 | 1.00 | 44.42 |
| ATOM | 3859 | CB | LYS | 510 | 74.069 | -3.259 | 5.365 | 1.00 | 46.34 |
| ATOM | 3860 | CG | LYS | 510 | 73.226 | -2.622 | 4.284 | 1.00 | 54.93 |
| ATOM | 3861 | CD | LYS | 510 | 73.825 | -2.807 | 2.899 | 1.00 | 58.33 |
| ATOM | 3862 | CE | LYS | 510 | 73.118 | -3.931 | 2.152 | 1.00 | 59.17 |
| ATOM | 3863 | NZ | LYS | 510 | 73.317 | -5.251 | 2.813 | 1.00 | 56.09 |
| ATOM | 3867 | C | LYS | 510 | 74.734 | -1.499 | 7.075 | 1.00 | 40.83 |
| ATOM | 3868 | O | LYS | 510 | 74.480 | -2.020 | 8.162 | 1.00 | 38.59 |
| ATOM | 3869 | N | VAL | 511 | 74.679 | -0.183 | 6.891 | 1.00 | 36.28 |
| ATOM | 3871 | CA | VAL | 511 | 74.265 | 0.720 | 7.957 | 1.00 | 31.41 |
| ATOM | 3872 | CB | VAL | 511 | 75.480 | 1.389 | 8.690 | 1.00 | 32.80 |
| ATOM | 3873 | CG1 | VAL | 511 | 76.315 | 0.346 | 9.420 | 1.00 | 29.97 |
| ATOM | 3874 | CG2 | VAL | 511 | 76.353 | 2.175 | 7.706 | 1.00 | 30.20 |
| ATOM | 3875 | C | VAL | 511 | 73.408 | 1.812 | 7.360 | 1.00 | 28.40 |
| ATOM | 3876 | O | VAL | 511 | 73.305 | 1.914 | 6.147 | 1.00 | 27.45 |
| ATOM | 3877 | N | ALA | 512 | 72.756 | 2.598 | 8.207 | 1.00 | 27.30 |
| ATOM | 3879 | CA | ALA | 512 | 71.953 | 3.701 | 7.715 | 1.00 | 26.66 |
| ATOM | 3880 | CB | ALA | 512 | 70.557 | 3.640 | 8.278 | 1.00 | 24.24 |
| ATOM | 3881 | C | ALA | 512 | 72.670 | 4.965 | 8.173 | 1.00 | 28.52 |
| ATOM | 3882 | O | ALA | 512 | 73.140 | 5.036 | 9.319 | 1.00 | 26.66 |
| ATOM | 3883 | N | VAL | 513 | 72.768 | 5.949 | 7.275 | 1.00 | 29.18 |
| ATOM | 3885 | CA | VAL | 513 | 73.442 | 7.217 | 7.569 | 1.00 | 29.65 |
| ATOM | 3886 | CB | VAL | 513 | 74.631 | 7.482 | 6.601 | 1.00 | 28.93 |
| ATOM | 3887 | CG1 | VAL | 513 | 75.384 | 8.722 | 7.015 | 1.00 | 25.51 |
| ATOM | 3888 | CG2 | VAL | 513 | 75.570 | 6.292 | 6.550 | 1.00 | 29.45 |
| ATOM | 3889 | C | VAL | 513 | 72.509 | 8.407 | 7.476 | 1.00 | 30.45 |
| ATOM | 3890 | O | VAL | 513 | 71.900 | 8.646 | 6.431 | 1.00 | 30.15 |
| ATOM | 3891 | N | LYS | 514 | 72.402 | 9.143 | 8.578 | 1.00 | 33.29 |
| ATOM | 3893 | CA | LYS | 514 | 71.575 | 10.357 | 8.654 | 1.00 | 33.28 |
| ATOM | 3894 | CB | LYS | 514 | 71.017 | 10.537 | 10.068 | 1.00 | 38.67 |
| ATOM | 3895 | CG | LYS | 514 | 70.074 | 9.456 | 10.531 | 1.00 | 45.73 |
| ATOM | 3896 | CD | LYS | 514 | 69.462 | 9.860 | 11.855 | 1.00 | 53.93 |
| ATOM | 3897 | CE | LYS | 514 | 68.450 | 8.840 | 12.337 | 1.00 | 63.59 |
| ATOM | 3898 | NZ | LYS | 514 | 67.206 | 8.823 | 11.517 | 1.00 | 71.90 |
| ATOM | 3902 | C | LYS | 514 | 72.451 | 11.568 | 8.312 | 1.00 | 29.45 |
| ATOM | 3903 | O | LYS | 514 | 73.584 | 11.673 | 8.794 | 1.00 | 25.64 |
| ATOM | 3904 | N | MET | 515 | 71.918 | 12.495 | 7.522 | 1.00 | 29.42 |
| ATOM | 3906 | CA | MET | 515 | 72.668 | 13.690 | 7.119 | 1.00 | 30.46 |
| ATOM | 3907 | CB | MET | 515 | 73.464 | 13.391 | 5.846 | 1.00 | 29.63 |
| ATOM | 3908 | CG | MET | 515 | 72.557 | 13.070 | 4.665 | 1.00 | 32.48 |
| ATOM | 3909 | SD | MET | 515 | 73.391 | 12.475 | 3.218 | 1.00 | 33.06 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3910 | CE | MET | 515 | 73.734 | 10.809 | 3.715 | 1.00 | 30.26 |
| ATOM | 3911 | C | MET | 515 | 71.700 | 14.839 | 6.848 | 1.00 | 30.75 |
| ATOM | 3912 | O | MET | 515 | 70.478 | 14.654 | 6.867 | 1.00 | 33.07 |
| ATOM | 3913 | N | LEU | 516 | 72.238 | 16.027 | 6.608 | 1.00 | 30.32 |
| ATOM | 3915 | CA | LEU | 516 | 71.414 | 17.194 | 6.304 | 1.00 | 30.21 |
| ATOM | 3916 | CB | LEU | 516 | 72.112 | 18.487 | 6.748 | 1.00 | 26.54 |
| ATOM | 3917 | CG | LEU | 516 | 72.452 | 18.668 | 8.227 | 1.00 | 23.97 |
| ATOM | 3918 | CD1 | LEU | 516 | 73.345 | 19.858 | 8.412 | 1.00 | 24.27 |
| ATOM | 3919 | CD2 | LEU | 516 | 71.198 | 18.850 | 9.023 | 1.00 | 21.46 |
| ATOM | 3920 | C | LEU | 516 | 71.197 | 17.265 | 4.800 | 1.00 | 33.44 |
| ATOM | 3921 | O | LEU | 516 | 72.016 | 16.784 | 4.015 | 1.00 | 34.50 |
| ATOM | 3922 | N | LYS | 517 | 70.082 | 17.863 | 4.400 | 1.00 | 36.36 |
| ATOM | 3924 | CA | LYS | 517 | 69.783 | 18.048 | 2.993 | 1.00 | 34.58 |
| ATOM | 3925 | CB | LYS | 517 | 68.281 | 18.255 | 2.784 | 1.00 | 38.96 |
| ATOM | 3926 | CG | LYS | 517 | 67.409 | 17.155 | 3.380 | 1.00 | 44.34 |
| ATOM | 3927 | CD | LYS | 517 | 66.128 | 16.920 | 2.572 | 1.00 | 52.11 |
| ATOM | 3928 | CE | LYS | 517 | 65.138 | 18.083 | 2.637 | 1.00 | 58.29 |
| ATOM | 3929 | NZ | LYS | 517 | 63.915 | 17.833 | 1.786 | 1.00 | 60.90 |
| ATOM | 3933 | C | LYS | 517 | 70.567 | 19.304 | 2.597 | 1.00 | 33.51 |
| ATOM | 3934 | O | LYS | 517 | 71.024 | 20.064 | 3.460 | 1.00 | 30.34 |
| ATOM | 3935 | N | SER | 518 | 70.701 | 19.539 | 1.296 | 1.00 | 34.39 |
| ATOM | 3937 | CA | SER | 518 | 71.444 | 20.693 | 0.788 | 1.00 | 35.84 |
| ATOM | 3938 | CB | SER | 518 | 71.537 | 20.618 | -0.731 | 1.00 | 33.66 |
| ATOM | 3939 | OG | SER | 518 | 70.282 | 20.258 | -1.266 | 1.00 | 38.73 |
| ATOM | 3941 | C | SER | 518 | 70.879 | 22.045 | 1.198 | 1.00 | 36.91 |
| ATOM | 3942 | O | SER | 518 | 71.591 | 23.050 | 1.205 | 1.00 | 37.32 |
| ATOM | 3943 | N | ASP | 519 | 69.598 | 22.069 | 1.538 | 1.00 | 37.88 |
| ATOM | 3945 | CA | ASP | 519 | 68.945 | 23.313 | 1.936 | 1.00 | 38.63 |
| ATOM | 3946 | CB | ASP | 519 | 67.517 | 23.364 | 1.375 | 1.00 | 42.23 |
| ATOM | 3947 | CG | ASP | 519 | 66.669 | 22.151 | 1.775 | 1.00 | 48.87 |
| ATOM | 3948 | OD1 | ASP | 519 | 67.070 | 21.380 | 2.681 | 1.00 | 49.21 |
| ATOM | 3949 | OD2 | ASP | 519 | 65.582 | 21.972 | 1.181 | 1.00 | 54.93 |
| ATOM | 3950 | C | ASP | 519 | 68.916 | 23.537 | 3.443 | 1.00 | 38.06 |
| ATOM | 3951 | O | ASP | 519 | 68.246 | 24.451 | 3.916 | 1.00 | 39.38 |
| ATOM | 3952 | N | ALA | 520 | 69.622 | 22.692 | 4.191 | 1.00 | 36.24 |
| ATOM | 3954 | CA | ALA | 520 | 69.631 | 22.795 | 5.648 | 1.00 | 34.69 |
| ATOM | 3955 | CB | ALA | 520 | 70.359 | 21.613 | 6.259 | 1.00 | 35.68 |
| ATOM | 3956 | C | ALA | 520 | 70.213 | 24.087 | 6.173 | 1.00 | 33.54 |
| ATOM | 3957 | O | ALA | 520 | 71.039 | 24.718 | 5.522 | 1.00 | 34.83 |
| ATOM | 3958 | N | THR | 521 | 69.815 | 24.452 | 7.384 | 1.00 | 34.45 |
| ATOM | 3960 | CA | THR | 521 | 70.315 | 25.668 | 8.001 | 1.00 | 36.51 |
| ATOM | 3961 | CB | THR | 521 | 69.148 | 26.592 | 8.493 | 1.00 | 39.14 |
| ATOM | 3962 | OG1 | THR | 521 | 68.529 | 26.031 | 9.659 | 1.00 | 41.61 |
| ATOM | 3964 | CG2 | THR | 521 | 68.081 | 26.750 | 7.409 | 1.00 | 40.14 |
| ATOM | 3965 | C | THR | 521 | 71.228 | 25.303 | 9.170 | 1.00 | 36.35 |
| ATOM | 3966 | O | THR | 521 | 71.376 | 24.125 | 9.510 | 1.00 | 32.23 |
| ATOM | 3967 | N | GLU | 522 | 71.868 | 26.310 | 9.756 | 1.00 | 39.33 |
| ATOM | 3969 | CA | GLU | 522 | 72.747 | 26.092 | 10.890 | 1.00 | 44.59 |
| ATOM | 3970 | CB | GLU | 522 | 73.364 | 27.424 | 11.335 | 1.00 | 51.80 |
| ATOM | 3971 | CG | GLU | 522 | 74.463 | 27.311 | 12.418 | 1.00 | 64.10 |
| ATOM | 3972 | CD | GLU | 522 | 75.811 | 26.815 | 11.886 | 1.00 | 69.12 |
| ATOM | 3973 | OE1 | GLU | 522 | 76.784 | 27.605 | 11.869 | 1.00 | 69.26 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3974 | OE2 | GLU | 522 | 75.900 | 25.629 | 11.502 | 1.00 | 73.62 |
| ATOM | 3975 | C | GLU | 522 | 71.953 | 25.447 | 12.042 | 1.00 | 44.53 |
| ATOM | 3976 | O | GLU | 522 | 72.482 | 24.617 | 12.786 | 1.00 | 44.95 |
| ATOM | 3977 | N | LYS | 523 | 70.679 | 25.814 | 12.167 | 1.00 | 42.99 |
| ATOM | 3979 | CA | LYS | 523 | 69.826 | 25.264 | 13.216 | 1.00 | 42.17 |
| ATOM | 3980 | CB | LYS | 523 | 68.519 | 26.053 | 13.329 | 1.00 | 45.99 |
| ATOM | 3981 | CG | LYS | 523 | 67.583 | 25.582 | 14.433 | 1.00 | 48.74 |
| ATOM | 3982 | CD | LYS | 523 | 66.296 | 25.027 | 13.832 | 1.00 | 57.24 |
| ATOM | 3983 | CE | LYS | 523 | 65.405 | 24.383 | 14.884 | 1.00 | 60.31 |
| ATOM | 3984 | NZ | LYS | 523 | 64.309 | 23.586 | 14.247 | 1.00 | 65.17 |
| ATOM | 3988 | C | LYS | 523 | 69.563 | 23.793 | 12.935 | 1.00 | 39.03 |
| ATOM | 3989 | O | LYS | 523 | 69.581 | 22.973 | 13.850 | 1.00 | 40.65 |
| ATOM | 3990 | N | ASP | 524 | 69.331 | 23.457 | 11.672 | 1.00 | 34.91 |
| ATOM | 3992 | CA | ASP | 524 | 69.122 | 22.068 | 11.294 | 1.00 | 33.12 |
| ATOM | 3993 | CB | ASP | 524 | 68.876 | 21.942 | 9.790 | 1.00 | 34.84 |
| ATOM | 3994 | CG | ASP | 524 | 67.482 | 22.352 | 9.389 | 1.00 | 36.47 |
| ATOM | 3995 | OD1 | ASP | 524 | 66.552 | 22.193 | 10.204 | 1.00 | 41.59 |
| ATOM | 3996 | OD2 | ASP | 524 | 67.307 | 22.815 | 8.248 | 1.00 | 38.19 |
| ATOM | 3997 | C | ASP | 524 | 70.383 | 21.284 | 11.653 | 1.00 | 33.94 |
| ATOM | 3998 | O | ASP | 524 | 70.301 | 20.154 | 12.139 | 1.00 | 37.40 |
| ATOM | 3999 | N | LEU | 525 | 71.554 | 21.869 | 11.404 | 1.00 | 32.39 |
| ATOM | 4001 | CA | LEU | 525 | 72.799 | 21.186 | 11.729 | 1.00 | 31.50 |
| ATOM | 4002 | CB | LEU | 525 | 74.018 | 21.998 | 11.278 | 1.00 | 29.05 |
| ATOM | 4003 | CG | LEU | 525 | 75.363 | 21.375 | 11.680 | 1.00 | 28.38 |
| ATOM | 4004 | CD1 | LEU | 525 | 75.521 | 19.990 | 11.065 | 1.00 | 27.27 |
| ATOM | 4005 | CD2 | LEU | 525 | 76.519 | 22.283 | 11.295 | 1.00 | 26.26 |
| ATOM | 4006 | C | LEU | 525 | 72.848 | 20.941 | 13.231 | 1.00 | 30.27 |
| ATOM | 4007 | O | LEU | 525 | 73.104 | 19.828 | 13.675 | 1.00 | 33.58 |
| ATOM | 4008 | N | SER | 526 | 72.563 | 21.982 | 14.000 | 1.00 | 29.63 |
| ATOM | 4010 | CA | SER | 526 | 72.544 | 21.914 | 15.459 | 1.00 | 30.26 |
| ATOM | 4011 | CB | SER | 526 | 72.046 | 23.251 | 16.013 | 1.00 | 32.03 |
| ATOM | 4012 | OG | SER | 526 | 71.923 | 23.199 | 17.417 | 1.00 | 37.02 |
| ATOM | 4014 | C | SER | 526 | 71.640 | 20.796 | 15.980 | 1.00 | 29.72 |
| ATOM | 4015 | O | SER | 526 | 71.924 | 20.162 | 16.998 | 1.00 | 27.54 |
| ATOM | 4016 | N | ASP | 527 | 70.525 | 20.588 | 15.291 | 1.00 | 28.97 |
| ATOM | 4018 | CA | ASP | 527 | 69.581 | 19.556 | 15.664 | 1.00 | 29.28 |
| ATOM | 4019 | CB | ASP | 527 | 68.289 | 19.710 | 14.855 | 1.00 | 29.08 |
| ATOM | 4020 | CG | ASP | 527 | 67.497 | 20.977 | 15.225 | 1.00 | 30.05 |
| ATOM | 4021 | OD1 | ASP | 527 | 67.750 | 21.597 | 16.292 | 1.00 | 24.32 |
| ATOM | 4022 | OD2 | ASP | 527 | 66.591 | 21.335 | 14.436 | 1.00 | 34.69 |
| ATOM | 4023 | C | ASP | 527 | 70.175 | 18.164 | 15.436 | 1.00 | 30.65 |
| ATOM | 4024 | O | ASP | 527 | 70.115 | 17.297 | 16.312 | 1.00 | 30.12 |
| ATOM | 4025 | N | LEU | 528 | 70.769 | 17.958 | 14.265 | 1.00 | 30.50 |
| ATOM | 4027 | CA | LEU | 528 | 71.358 | 16.669 | 13.946 | 1.00 | 29.54 |
| ATOM | 4028 | CB | LEU | 528 | 71.850 | 16.647 | 12.487 | 1.00 | 26.03 |
| ATOM | 4029 | CG | LEU | 528 | 72.409 | 15.320 | 11.942 | 1.00 | 24.26 |
| ATOM | 4030 | CD1 | LEU | 528 | 71.466 | 14.142 | 12.259 | 1.00 | 21.51 |
| ATOM | 4031 | CD2 | LEU | 528 | 72.644 | 15.437 | 10.450 | 1.00 | 15.05 |
| ATOM | 4032 | C | LEU | 528 | 72.494 | 16.342 | 14.933 | 1.00 | 30.51 |
| ATOM | 4033 | O | LEU | 528 | 72.641 | 15.192 | 15.354 | 1.00 | 29.79 |
| ATOM | 4034 | N | ILE | 529 | 73.281 | 17.351 | 15.305 | 1.00 | 30.86 |
| ATOM | 4036 | CA | ILE | 529 | 74.367 | 17.138 | 16.253 | 1.00 | 28.41 |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4037 | CB | ILE | 529 | 75.266 | 18.349 | 16.406 | 1.00 | 24.75 | |
| ATOM | 4038 | CG2 | ILE | 529 | 76.355 | 18.064 | 17.432 | 1.00 | 25.51 | |
| ATOM | 4039 | CG1 | ILE | 529 | 75.901 | 18.710 | 15.084 | 1.00 | 17.82 | |
| ATOM | 4040 | CD1 | ILE | 529 | 76.912 | 19.806 | 15.251 | 1.00 | 18.14 | |
| ATOM | 4041 | C | ILE | 529 | 73.821 | 16.813 | 17.641 | 1.00 | 30.17 | |
| ATOM | 4042 | O | ILE | 529 | 74.286 | 15.873 | 18.285 | 1.00 | 30.11 | |
| ATOM | 4043 | N | SER | 530 | 72.836 | 17.574 | 18.101 | 1.00 | 30.29 | |
| ATOM | 4045 | CA | SER | 530 | 72.271 | 17.310 | 19.418 | 1.00 | 33.14 | |
| ATOM | 4046 | CB | SER | 530 | 71.158 | 18.293 | 19.735 | 1.00 | 36.09 | |
| ATOM | 4047 | OG | SER | 530 | 70.224 | 18.323 | 18.670 | 1.00 | 49.01 | |
| ATOM | 4049 | C | SER | 530 | 71.740 | 15.881 | 19.479 | 1.00 | 33.80 | |
| ATOM | 4050 | O | SER | 530 | 71.896 | 15.190 | 20.492 | 1.00 | 37.06 | |
| ATOM | 4051 | N | GLU | 531 | 71.156 | 15.413 | 18.378 | 1.00 | 30.13 | |
| ATOM | 4053 | CA | GLU | 531 | 70.629 | 14.065 | 18.351 | 1.00 | 29.18 | |
| ATOM | 4054 | CB | GLU | 531 | 69.822 | 13.801 | 17.087 | 1.00 | 32.42 | |
| ATOM | 4055 | CG | GLU | 531 | 69.253 | 12.394 | 17.058 | 1.00 | 33.35 | |
| ATOM | 4056 | CD | GLU | 531 | 68.354 | 12.131 | 15.883 | 1.00 | 34.76 | |
| ATOM | 4057 | OE1 | GLU | 531 | 67.481 | 11.249 | 16.002 | 1.00 | 40.42 | |
| ATOM | 4058 | OE2 | GLU | 531 | 68.516 | 12.793 | 14.847 | 1.00 | 35.88 | |
| ATOM | 4059 | C | GLU | 531 | 71.734 | 13.025 | 18.488 | 1.00 | 28.27 | |
| ATOM | 4060 | O | GLU | 531 | 71.569 | 12.032 | 19.192 | 1.00 | 26.75 | |
| ATOM | 4061 | N | MET | 532 | 72.842 | 13.235 | 17.786 | 1.00 | 27.80 | |
| ATOM | 4063 | CA | MET | 532 | 73.976 | 12.320 | 17.835 | 1.00 | 27.82 | |
| ATOM | 4064 | CB | MET | 532 | 75.080 | 12.813 | 16.890 | 1.00 | 29.43 | |
| ATOM | 4065 | CG | MET | 532 | 76.461 | 12.225 | 17.138 | 1.00 | 24.34 | |
| ATOM | 4066 | SD | MET | 532 | 77.641 | 12.702 | 15.840 | 1.00 | 27.83 | |
| ATOM | 4067 | CE | MET | 532 | 77.791 | 14.462 | 16.193 | 1.00 | 21.90 | |
| ATOM | 4068 | C | MET | 532 | 74.499 | 12.272 | 19.260 | 1.00 | 29.53 | |
| ATOM | 4069 | O | MET | 532 | 74.742 | 11.197 | 19.809 | 1.00 | 30.14 | |
| ATOM | 4070 | N | GLU | 533 | 74.610 | 13.445 | 19.871 | 1.00 | 30.25 | |
| ATOM | 4072 | CA | GLU | 533 | 75.109 | 13.570 | 21.233 | 1.00 | 31.95 | |
| ATOM | 4073 | CB | GLU | 533 | 75.300 | 15.039 | 21.594 | 1.00 | 32.55 | |
| ATOM | 4074 | CG | GLU | 533 | 76.391 | 15.724 | 20.765 | 1.00 | 35.71 | |
| ATOM | 4075 | CD | GLU | 533 | 77.766 | 15.087 | 20.951 | 1.00 | 36.71 | |
| ATOM | 4076 | OE1 | GLU | 533 | 78.297 | 15.136 | 22.084 | 1.00 | 40.19 | |
| ATOM | 4077 | OE2 | GLU | 533 | 78.322 | 14.555 | 19.969 | 1.00 | 33.99 | |
| ATOM | 4078 | C | GLU | 533 | 74.185 | 12.886 | 22.225 | 1.00 | 33.06 | |
| ATOM | 4079 | O | GLU | 533 | 74.642 | 12.197 | 23.147 | 1.00 | 33.49 | |
| ATOM | 4080 | N | MET | 534 | 72.883 | 13.052 | 22.025 | 1.00 | 33.12 | |
| ATOM | 4082 | CA | MET | 534 | 71.913 | 12.432 | 22.900 | 1.00 | 32.48 | |
| ATOM | 4083 | CB | MET | 534 | 70.484 | 12.859 | 22.533 | 1.00 | 30.60 | |
| ATOM | 4084 | CG | MET | 534 | 69.591 | 12.915 | 23.791 | 0.50 | 28.70 | PRT1 |
| ATOM | 4085 | SD | MET | 534 | 67.787 | 12.849 | 23.608 | 0.50 | 27.55 | PRT1 |
| ATOM | 4086 | CE | MET | 534 | 67.409 | 14.560 | 23.291 | 0.50 | 26.84 | PRT1 |
| ATOM | 4087 | C | MET | 534 | 72.102 | 10.908 | 22.785 | 1.00 | 31.10 | |
| ATOM | 4088 | O | MET | 534 | 72.258 | 10.224 | 23.791 | 1.00 | 32.80 | |
| ATOM | 4089 | N | MET | 535 | 72.194 | 10.394 | 21.563 | 1.00 | 30.50 | |
| ATOM | 4091 | CA | MET | 535 | 72.399 | 8.961 | 21.368 | 1.00 | 29.25 | |
| ATOM | 4092 | CB | MET | 535 | 72.577 | 8.623 | 19.884 | 1.00 | 28.10 | |
| ATOM | 4093 | CG | MET | 535 | 71.337 | 8.876 | 19.042 | 1.00 | 27.48 | |
| ATOM | 4094 | SD | MET | 535 | 71.377 | 7.980 | 17.502 | 1.00 | 26.94 | |
| ATOM | 4095 | CE | MET | 535 | 71.346 | 9.275 | 16.310 | 1.00 | 33.72 | |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4096 | C | MET | 535 | 73.621 | 8.514 | 22.155 | 1.00 | 29.29 |
| ATOM | 4097 | O | MET | 535 | 73.640 | 7.412 | 22.710 | 1.00 | 29.06 |
| ATOM | 4098 | N | LYS | 536 | 74.644 | 9.367 | 22.185 | 1.00 | 31.75 |
| ATOM | 4100 | CA | LYS | 536 | 75.869 | 9.073 | 22.930 | 1.00 | 33.24 |
| ATOM | 4101 | CB | LYS | 536 | 76.950 | 10.108 | 22.628 | 1.00 | 31.29 |
| ATOM | 4102 | CG | LYS | 536 | 77.602 | 10.007 | 21.258 | 1.00 | 31.09 |
| ATOM | 4103 | CD | LYS | 536 | 78.570 | 11.154 | 21.103 | 1.00 | 28.76 |
| ATOM | 4104 | CE | LYS | 536 | 79.219 | 11.220 | 19.755 | 1.00 | 26.70 |
| ATOM | 4105 | NZ | LYS | 536 | 80.059 | 12.461 | 19.742 | 1.00 | 27.38 |
| ATOM | 4109 | C | LYS | 536 | 75.630 | 9.014 | 24.451 | 1.00 | 35.30 |
| ATOM | 4110 | O | LYS | 536 | 76.201 | 8.172 | 25.137 | 1.00 | 35.61 |
| ATOM | 4111 | N | MET | 537 | 74.788 | 9.902 | 24.972 | 1.00 | 35.67 |
| ATOM | 4113 | CA | MET | 537 | 74.517 | 9.908 | 26.408 | 1.00 | 38.27 |
| ATOM | 4114 | CB | MET | 537 | 73.858 | 11.221 | 26.844 | 1.00 | 43.86 |
| ATOM | 4115 | CG | MET | 537 | 74.801 | 12.420 | 26.884 | 1.00 | 55.46 |
| ATOM | 4116 | SD | MET | 537 | 76.189 | 12.272 | 28.062 | 1.00 | 63.44 |
| ATOM | 4117 | CE | MET | 537 | 75.383 | 12.822 | 29.591 | 1.00 | 62.14 |
| ATOM | 4118 | C | MET | 537 | 73.657 | 8.734 | 26.845 | 1.00 | 37.10 |
| ATOM | 4119 | O | MET | 537 | 73.855 | 8.188 | 27.920 | 1.00 | 39.26 |
| ATOM | 4120 | N | ILE | 538 | 72.723 | 8.320 | 26.003 | 1.00 | 34.96 |
| ATOM | 4122 | CA | ILE | 538 | 71.819 | 7.219 | 26.320 | 1.00 | 32.78 |
| ATOM | 4123 | CB | ILE | 538 | 70.618 | 7.202 | 25.342 | 1.00 | 32.48 |
| ATOM | 4124 | CG2 | ILE | 538 | 69.782 | 5.943 | 25.537 | 1.00 | 32.27 |
| ATOM | 4125 | CG1 | ILE | 538 | 69.756 | 8.449 | 25.538 | 1.00 | 31.77 |
| ATOM | 4126 | CD1 | ILE | 538 | 68.746 | 8.651 | 24.409 | 1.00 | 34.25 |
| ATOM | 4127 | C | ILE | 538 | 72.456 | 5.823 | 26.365 | 1.00 | 30.54 |
| ATOM | 4128 | O | ILE | 538 | 72.146 | 5.039 | 27.250 | 1.00 | 33.37 |
| ATOM | 4129 | N | GLY | 539 | 73.293 | 5.481 | 25.399 | 1.00 | 27.09 |
| ATOM | 4131 | CA | GLY | 539 | 73.892 | 4.162 | 25.419 | 1.00 | 28.72 |
| ATOM | 4132 | C | GLY | 539 | 73.173 | 3.135 | 24.552 | 1.00 | 31.16 |
| ATOM | 4133 | O | GLY | 539 | 72.069 | 3.379 | 24.060 | 1.00 | 32.94 |
| ATOM | 4134 | N | LYS | 540 | 73.808 | 1.981 | 24.370 | 1.00 | 31.68 |
| ATOM | 4136 | CA | LYS | 540 | 73.264 | 0.912 | 23.537 | 1.00 | 34.64 |
| ATOM | 4137 | CB | LYS | 540 | 74.399 | 0.032 | 23.029 | 1.00 | 33.47 |
| ATOM | 4138 | CG | LYS | 540 | 75.331 | 0.730 | 22.095 | 1.00 | 39.67 |
| ATOM | 4139 | CD | LYS | 540 | 76.396 | -0.209 | 21.573 | 1.00 | 41.48 |
| ATOM | 4140 | CE | LYS | 540 | 77.228 | 0.475 | 20.501 | 1.00 | 48.72 |
| ATOM | 4141 | NZ | LYS | 540 | 76.442 | 0.800 | 19.254 | 1.00 | 54.86 |
| ATOM | 4145 | C | LYS | 540 | 72.206 | -0.010 | 24.143 | 1.00 | 36.68 |
| ATOM | 4146 | O | LYS | 540 | 72.276 | -0.370 | 25.324 | 1.00 | 41.03 |
| ATOM | 4147 | N | HIS | 541 | 71.233 | -0.396 | 23.319 | 1.00 | 35.61 |
| ATOM | 4149 | CA | HIS | 541 | 70.190 | -1.335 | 23.711 | 1.00 | 34.24 |
| ATOM | 4150 | CB | HIS | 541 | 69.074 | -0.702 | 24.526 | 1.00 | 33.44 |
| ATOM | 4151 | CG | HIS | 541 | 68.118 | -1.711 | 25.083 | 1.00 | 34.60 |
| ATOM | 4152 | CD2 | HIS | 541 | 68.059 | -2.310 | 26.292 | 1.00 | 33.77 |
| ATOM | 4153 | ND1 | HIS | 541 | 67.143 | -2.316 | 24.309 | 1.00 | 34.19 |
| ATOM | 4155 | CE1 | HIS | 541 | 66.539 | -3.248 | 25.020 | 1.00 | 36.87 |
| ATOM | 4156 | NE2 | HIS | 541 | 67.074 | -3.272 | 26.228 | 1.00 | 34.05 |
| ATOM | 4158 | C | HIS | 541 | 69.624 | -2.023 | 22.474 | 1.00 | 36.31 |
| ATOM | 4159 | O | HIS | 541 | 69.342 | -1.378 | 21.457 | 1.00 | 38.40 |
| ATOM | 4160 | N | LYS | 542 | 69.407 | -3.331 | 22.586 | 1.00 | 36.42 |
| ATOM | 4162 | CA | LYS | 542 | 68.923 | -4.155 | 21.469 | 1.00 | 35.10 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4163 | CB | LYS | 542 | 68.680 | -5.602 | 21.915 | 1.00 | 34.24 |
| ATOM | 4164 | C | LYS | 542 | 67.674 | -3.646 | 20.802 | 1.00 | 32.40 |
| ATOM | 4165 | O | LYS | 542 | 67.507 | -3.822 | 19.612 | 1.00 | 32.37 |
| ATOM | 4166 | N | ASN | 543 | 66.785 | -3.046 | 21.580 | 1.00 | 32.12 |
| ATOM | 4168 | CA | ASN | 543 | 65.541 | -2.561 | 21.015 | 1.00 | 33.01 |
| ATOM | 4169 | CB | ASN | 543 | 64.361 | -3.081 | 21.842 | 1.00 | 34.26 |
| ATOM | 4170 | CG | ASN | 543 | 64.365 | -4.597 | 21.979 | 1.00 | 32.20 |
| ATOM | 4171 | OD1 | ASN | 543 | 64.633 | -5.128 | 23.050 | 1.00 | 32.23 |
| ATOM | 4172 | ND2 | ASN | 543 | 64.077 | -5.292 | 20.904 | 1.00 | 30.50 |
| ATOM | 4175 | C | ASN | 543 | 65.424 | -1.050 | 20.719 | 1.00 | 32.21 |
| ATOM | 4176 | O | ASN | 543 | 64.326 | -0.481 | 20.765 | 1.00 | 31.13 |
| ATOM | 4177 | N | ILE | 544 | 66.556 | -0.419 | 20.397 | 1.00 | 30.52 |
| ATOM | 4179 | CA | ILE | 544 | 66.611 | 1.002 | 20.028 | 1.00 | 29.01 |
| ATOM | 4180 | CB | ILE | 544 | 67.040 | 1.962 | 21.208 | 1.00 | 25.83 |
| ATOM | 4181 | CG2 | ILE | 544 | 66.244 | 1.682 | 22.467 | 1.00 | 24.46 |
| ATOM | 4182 | CG1 | ILE | 544 | 68.532 | 1.848 | 21.522 | 1.00 | 27.54 |
| ATOM | 4183 | CD1 | ILE | 544 | 69.008 | 2.839 | 22.581 | 1.00 | 22.70 |
| ATOM | 4184 | C | ILE | 544 | 67.617 | 1.118 | 18.870 | 1.00 | 29.49 |
| ATOM | 4185 | O | ILE | 544 | 68.410 | 0.194 | 18.633 | 1.00 | 27.26 |
| ATOM | 4186 | N | ILE | 545 | 67.504 | 2.184 | 18.078 | 1.00 | 28.74 |
| ATOM | 4188 | CA | ILE | 545 | 68.453 | 2.396 | 16.992 | 1.00 | 27.06 |
| ATOM | 4189 | CB | ILE | 545 | 67.913 | 3.350 | 15.921 | 1.00 | 23.64 |
| ATOM | 4190 | CG2 | ILE | 545 | 69.027 | 3.727 | 14.955 | 1.00 | 23.96 |
| ATOM | 4191 | CG1 | ILE | 545 | 66.754 | 2.692 | 15.167 | 1.00 | 23.13 |
| ATOM | 4192 | CD1 | ILE | 545 | 67.152 | 1.481 | 14.339 | 1.00 | 20.61 |
| ATOM | 4193 | C | ILE | 545 | 69.720 | 2.968 | 17.633 | 1.00 | 26.93 |
| ATOM | 4194 | O | ILE | 545 | 69.719 | 4.075 | 18.160 | 1.00 | 28.63 |
| ATOM | 4195 | N | ASN | 546 | 70.800 | 2.200 | 17.560 | 1.00 | 28.53 |
| ATOM | 4197 | CA | ASN | 546 | 72.075 | 2.567 | 18.161 | 1.00 | 29.39 |
| ATOM | 4198 | CB | ASN | 546 | 72.752 | 1.308 | 18.718 | 1.00 | 29.14 |
| ATOM | 4199 | CG | ASN | 546 | 71.908 | 0.613 | 19.772 | 1.00 | 30.21 |
| ATOM | 4200 | OD1 | ASN | 546 | 71.804 | 1.088 | 20.899 | 1.00 | 30.74 |
| ATOM | 4201 | ND2 | ASN | 546 | 71.290 | -0.505 | 19.406 | 1.00 | 30.79 |
| ATOM | 4204 | C | ASN | 546 | 73.034 | 3.303 | 17.238 | 1.00 | 30.78 |
| ATOM | 4205 | O | ASN | 546 | 73.011 | 3.126 | 16.015 | 1.00 | 33.04 |
| ATOM | 4206 | N | LEU | 547 | 73.866 | 4.151 | 17.837 | 1.00 | 31.07 |
| ATOM | 4208 | CA | LEU | 547 | 74.880 | 4.904 | 17.101 | 1.00 | 31.37 |
| ATOM | 4209 | CB | LEU | 547 | 75.284 | 6.165 | 17.875 | 1.00 | 27.32 |
| ATOM | 4210 | CG | LEU | 547 | 76.413 | 7.032 | 17.297 | 1.00 | 24.17 |
| ATOM | 4211 | CD1 | LEU | 547 | 75.953 | 7.768 | 16.069 | 1.00 | 18.06 |
| ATOM | 4212 | CD2 | LEU | 547 | 76.864 | 8.014 | 18.348 | 1.00 | 22.50 |
| ATOM | 4213 | C | LEU | 547 | 76.107 | 3.999 | 16.861 | 1.00 | 33.38 |
| ATOM | 4214 | O | LEU | 547 | 76.610 | 3.343 | 17.789 | 1.00 | 33.58 |
| ATOM | 4215 | N | LEU | 548 | 76.543 | 3.919 | 15.607 | 1.00 | 32.72 |
| ATOM | 4217 | CA | LEU | 548 | 77.694 | 3.104 | 15.259 | 1.00 | 31.50 |
| ATOM | 4218 | CB | LEU | 548 | 77.388 | 2.244 | 14.029 | 1.00 | 26.30 |
| ATOM | 4219 | CG | LEU | 548 | 76.148 | 1.341 | 14.158 | 1.00 | 25.93 |
| ATOM | 4220 | CD1 | LEU | 548 | 76.034 | 0.513 | 12.906 | 1.00 | 28.37 |
| ATOM | 4221 | CD2 | LEU | 548 | 76.196 | 0.436 | 15.394 | 1.00 | 15.84 |
| ATOM | 4222 | C | LEU | 548 | 78.941 | 3.965 | 15.030 | 1.00 | 33.69 |
| ATOM | 4223 | O | LEU | 548 | 80.063 | 3.488 | 15.167 | 1.00 | 37.41 |
| ATOM | 4224 | N | GLY | 549 | 78.746 | 5.229 | 14.675 | 1.00 | 34.10 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4226 | CA | GLY | 549 | 79.871 | 6.116 | 14.454 | 1.00 | 31.50 |
| ATOM | 4227 | C | GLY | 549 | 79.425 | 7.429 | 13.839 | 1.00 | 31.11 |
| ATOM | 4228 | O | GLY | 549 | 78.221 | 7.686 | 13.700 | 1.00 | 30.15 |
| ATOM | 4229 | N | ALA | 550 | 80.388 | 8.268 | 13.474 | 1.00 | 31.02 |
| ATOM | 4231 | CA | ALA | 550 | 80.074 | 9.540 | 12.850 | 1.00 | 29.00 |
| ATOM | 4232 | CB | ALA | 550 | 79.537 | 10.526 | 13.899 | 1.00 | 27.87 |
| ATOM | 4233 | C | ALA | 550 | 81.257 | 10.149 | 12.102 | 1.00 | 27.66 |
| ATOM | 4234 | O | ALA | 550 | 82.422 | 9.942 | 12.474 | 1.00 | 25.24 |
| ATOM | 4235 | N | CYS | 551 | 80.944 | 10.810 | 10.984 | 1.00 | 27.61 |
| ATOM | 4237 | CA | CYS | 551 | 81.924 | 11.540 | 10.170 | 1.00 | 25.02 |
| ATOM | 4238 | CB | CYS | 551 | 81.754 | 11.237 | 8.680 | 1.00 | 22.41 |
| ATOM | 4239 | SG | CYS | 551 | 82.155 | 9.553 | 8.187 | 1.00 | 27.24 |
| ATOM | 4240 | C | CYS | 551 | 81.583 | 13.009 | 10.447 | 1.00 | 24.31 |
| ATOM | 4241 | O | CYS | 551 | 80.569 | 13.525 | 9.958 | 1.00 | 23.55 |
| ATOM | 4242 | N | THR | 552 | 82.367 | 13.657 | 11.303 | 1.00 | 23.22 |
| ATOM | 4244 | CA | THR | 552 | 82.110 | 15.046 | 11.664 | 1.00 | 25.73 |
| ATOM | 4245 | CB | THR | 552 | 82.138 | 15.215 | 13.202 | 1.00 | 26.50 |
| ATOM | 4246 | OG1 | THR | 552 | 83.479 | 15.031 | 13.664 | 1.00 | 26.31 |
| ATOM | 4248 | CG2 | THR | 552 | 81.257 | 14.171 | 13.886 | 1.00 | 26.64 |
| ATOM | 4249 | C | THR | 552 | 83.134 | 16.014 | 11.090 | 1.00 | 27.93 |
| ATOM | 4250 | O | THR | 552 | 82.894 | 17.216 | 11.005 | 1.00 | 28.35 |
| ATOM | 4251 | N | GLN | 553 | 84.264 | 15.473 | 10.663 | 1.00 | 30.26 |
| ATOM | 4253 | CA | GLN | 553 | 85.355 | 16.288 | 10.153 | 1.00 | 29.27 |
| ATOM | 4254 | CB | GLN | 553 | 86.669 | 15.768 | 10.763 | 1.00 | 29.54 |
| ATOM | 4255 | CG | GLN | 553 | 86.653 | 15.655 | 12.288 | 1.00 | 28.00 |
| ATOM | 4256 | CD | GLN | 553 | 86.534 | 17.007 | 12.981 | 1.00 | 26.86 |
| ATOM | 4257 | OE1 | GLN | 553 | 87.440 | 17.821 | 12.902 | 1.00 | 30.85 |
| ATOM | 4258 | NE2 | GLN | 553 | 85.421 | 17.239 | 13.676 | 1.00 | 23.89 |
| ATOM | 4261 | C | GLN | 553 | 85.475 | 16.316 | 8.634 | 1.00 | 28.30 |
| ATOM | 4262 | O | GLN | 553 | 85.221 | 15.313 | 7.967 | 1.00 | 31.00 |
| ATOM | 4263 | N | ASP | 554 | 85.860 | 17.480 | 8.119 | 1.00 | 26.89 |
| ATOM | 4265 | CA | ASP | 554 | 86.070 | 17.725 | 6.695 | 1.00 | 27.85 |
| ATOM | 4266 | CB | ASP | 554 | 87.370 | 17.081 | 6.257 | 1.00 | 33.44 |
| ATOM | 4267 | CG | ASP | 554 | 88.534 | 17.564 | 7.060 | 1.00 | 37.63 |
| ATOM | 4268 | OD1 | ASP | 554 | 89.038 | 18.664 | 6.763 | 1.00 | 42.66 |
| ATOM | 4269 | OD2 | ASP | 554 | 88.929 | 16.843 | 8.000 | 1.00 | 35.80 |
| ATOM | 4270 | C | ASP | 554 | 84.976 | 17.341 | 5.715 | 1.00 | 28.04 |
| ATOM | 4271 | O | ASP | 554 | 85.193 | 16.518 | 4.826 | 1.00 | 31.06 |
| ATOM | 4272 | N | GLY | 555 | 83.824 | 17.981 | 5.842 | 1.00 | 28.26 |
| ATOM | 4274 | CA | GLY | 555 | 82.720 | 17.694 | 4.949 | 1.00 | 25.89 |
| ATOM | 4275 | C | GLY | 555 | 81.438 | 17.567 | 5.734 | 1.00 | 23.07 |
| ATOM | 4276 | O | GLY | 555 | 81.423 | 17.795 | 6.941 | 1.00 | 20.20 |
| ATOM | 4277 | N | PRO | 556 | 80.338 | 17.185 | 5.076 | 1.00 | 22.81 |
| ATOM | 4278 | CD | PRO | 556 | 80.280 | 16.750 | 3.679 | 1.00 | 22.33 |
| ATOM | 4279 | CA | PRO | 556 | 79.039 | 17.032 | 5.733 | 1.00 | 23.99 |
| ATOM | 4280 | CB | PRO | 556 | 78.154 | 16.499 | 4.612 | 1.00 | 22.41 |
| ATOM | 4281 | CG | PRO | 556 | 79.144 | 15.801 | 3.698 | 1.00 | 24.36 |
| ATOM | 4282 | C | PRO | 556 | 79.080 | 16.066 | 6.911 | 1.00 | 26.98 |
| ATOM | 4283 | O | PRO | 556 | 79.854 | 15.111 | 6.934 | 1.00 | 28.57 |
| ATOM | 4284 | N | LEU | 557 | 78.237 | 16.325 | 7.896 | 1.00 | 29.25 |
| ATOM | 4286 | CA | LEU | 557 | 78.168 | 15.471 | 9.070 | 1.00 | 30.83 |
| ATOM | 4287 | CB | LEU | 557 | 77.550 | 16.225 | 10.251 | 1.00 | 33.20 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4288 | CG | LEU | 557 | 77.109 | 15.416 | 11.475 | 1.00 | 30.01 |
| ATOM | 4289 | CD1 | LEU | 557 | 78.304 | 14.793 | 12.174 | 1.00 | 29.05 |
| ATOM | 4290 | CD2 | LEU | 557 | 76.365 | 16.341 | 12.407 | 1.00 | 29.20 |
| ATOM | 4291 | C | LEU | 557 | 77.324 | 14.238 | 8.780 | 1.00 | 30.33 |
| ATOM | 4292 | O | LEU | 557 | 76.175 | 14.343 | 8.330 | 1.00 | 27.66 |
| ATOM | 4293 | N | TYR | 558 | 77.913 | 13.071 | 9.002 | 1.00 | 30.68 |
| ATOM | 4295 | CA | TYR | 558 | 77.214 | 11.823 | 8.812 | 1.00 | 29.26 |
| ATOM | 4296 | CB | TYR | 558 | 77.978 | 10.933 | 7.840 | 1.00 | 30.99 |
| ATOM | 4297 | CG | TYR | 558 | 78.066 | 11.481 | 6.430 | 1.00 | 35.01 |
| ATOM | 4298 | CD1 | TYR | 558 | 79.108 | 11.109 | 5.592 | 1.00 | 36.17 |
| ATOM | 4299 | CE1 | TYR | 558 | 79.198 | 11.600 | 4.296 | 1.00 | 41.40 |
| ATOM | 4300 | CD2 | TYR | 558 | 77.109 | 12.368 | 5.941 | 1.00 | 36.44 |
| ATOM | 4301 | CE2 | TYR | 558 | 77.188 | 12.871 | 4.648 | 1.00 | 40.96 |
| ATOM | 4302 | CZ | TYR | 558 | 78.237 | 12.484 | 3.825 | 1.00 | 43.59 |
| ATOM | 4303 | OH | TYR | 558 | 78.298 | 12.965 | 2.525 | 1.00 | 42.91 |
| ATOM | 4305 | C | TYR | 558 | 77.081 | 11.125 | 10.164 | 1.00 | 28.18 |
| ATOM | 4306 | O | TYR | 558 | 78.077 | 10.855 | 10.835 | 1.00 | 28.06 |
| ATOM | 4307 | N | VAL | 559 | 75.842 | 10.879 | 10.574 | 1.00 | 26.72 |
| ATOM | 4309 | CA | VAL | 559 | 75.548 | 10.175 | 11.821 | 1.00 | 26.72 |
| ATOM | 4310 | CB | VAL | 559 | 74.326 | 10.813 | 12.552 | 1.00 | 28.03 |
| ATOM | 4311 | CG1 | VAL | 559 | 73.915 | 9.992 | 13.771 | 1.00 | 29.85 |
| ATOM | 4312 | CG2 | VAL | 559 | 74.655 | 12.236 | 12.982 | 1.00 | 29.37 |
| ATOM | 4313 | C | VAL | 559 | 75.238 | 8.723 | 11.443 | 1.00 | 25.58 |
| ATOM | 4314 | O | VAL | 559 | 74.131 | 8.402 | 10.988 | 1.00 | 25.73 |
| ATOM | 4315 | N | ILE | 560 | 76.214 | 7.851 | 11.642 | 1.00 | 24.35 |
| ATOM | 4317 | CA | ILE | 560 | 76.061 | 6.448 | 11.281 | 1.00 | 26.64 |
| ATOM | 4318 | CB | ILE | 560 | 77.441 | 5.781 | 11.002 | 1.00 | 26.53 |
| ATOM | 4319 | CG2 | ILE | 560 | 77.252 | 4.359 | 10.465 | 1.00 | 27.80 |
| ATOM | 4320 | CG1 | ILE | 560 | 78.254 | 6.620 | 10.004 | 1.00 | 24.69 |
| ATOM | 4321 | CD1 | ILE | 560 | 79.671 | 6.112 | 9.763 | 1.00 | 17.05 |
| ATOM | 4322 | C | ILE | 560 | 75.312 | 5.633 | 12.339 | 1.00 | 27.95 |
| ATOM | 4323 | O | ILE | 560 | 75.777 | 5.493 | 13.479 | 1.00 | 25.16 |
| ATOM | 4324 | N | VAL | 561 | 74.163 | 5.084 | 11.951 | 1.00 | 27.43 |
| ATOM | 4326 | CA | VAL | 561 | 73.352 | 4.265 | 12.847 | 1.00 | 27.69 |
| ATOM | 4327 | CB | VAL | 561 | 72.048 | 5.000 | 13.251 | 1.00 | 25.08 |
| ATOM | 4328 | CG1 | VAL | 561 | 72.367 | 6.302 | 13.936 | 1.00 | 19.97 |
| ATOM | 4329 | CG2 | VAL | 561 | 71.186 | 5.250 | 12.033 | 1.00 | 25.55 |
| ATOM | 4330 | C | VAL | 561 | 73.031 | 2.896 | 12.202 | 1.00 | 30.21 |
| ATOM | 4331 | O | VAL | 561 | 73.404 | 2.623 | 11.045 | 1.00 | 32.04 |
| ATOM | 4332 | N | GLU | 562 | 72.306 | 2.062 | 12.944 | 1.00 | 28.88 |
| ATOM | 4334 | CA | GLU | 562 | 71.940 | 0.714 | 12.509 | 1.00 | 27.69 |
| ATOM | 4335 | CB | GLU | 562 | 71.448 | -0.081 | 13.712 | 1.00 | 26.79 |
| ATOM | 4336 | CG | GLU | 562 | 72.387 | 0.001 | 14.873 | 1.00 | 28.13 |
| ATOM | 4337 | CD | GLU | 562 | 72.012 | -0.916 | 16.003 | 1.00 | 31.86 |
| ATOM | 4338 | OE1 | GLU | 562 | 72.772 | -1.876 | 16.255 | 1.00 | 33.17 |
| ATOM | 4339 | OE2 | GLU | 562 | 70.974 | -0.654 | 16.639 | 1.00 | 35.50 |
| ATOM | 4340 | C | GLU | 562 | 70.898 | 0.636 | 11.405 | 1.00 | 27.34 |
| ATOM | 4341 | O | GLU | 562 | 69.990 | 1.453 | 11.358 | 1.00 | 29.72 |
| ATOM | 4342 | N | TYR | 563 | 71.002 | -0.392 | 10.568 | 1.00 | 28.07 |
| ATOM | 4344 | CA | TYR | 563 | 70.080 | -0.626 | 9.455 | 1.00 | 32.50 |
| ATOM | 4345 | CB | TYR | 563 | 70.848 | -1.236 | 8.269 | 1.00 | 28.32 |
| ATOM | 4346 | CG | TYR | 563 | 70.042 | -1.427 | 7.007 | 1.00 | 26.56 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4347 | CD1 | TYR | 563 | 69.338 | -0.378 | 6.448 | 1.00 | 30.49 |
| ATOM | 4348 | CE1 | TYR | 563 | 68.620 | -0.536 | 5.258 | 1.00 | 32.83 |
| ATOM | 4349 | CD2 | TYR | 563 | 70.011 | -2.652 | 6.350 | 1.00 | 29.07 |
| ATOM | 4350 | CE2 | TYR | 563 | 69.300 | -2.821 | 5.151 | 1.00 | 30.70 |
| ATOM | 4351 | CZ | TYR | 563 | 68.605 | -1.755 | 4.619 | 1.00 | 33.54 |
| ATOM | 4352 | OH | TYR | 563 | 67.876 | -1.919 | 3.460 | 1.00 | 40.20 |
| ATOM | 4354 | C | TYR | 563 | 68.930 | -1.564 | 9.878 | 1.00 | 36.30 |
| ATOM | 4355 | O | TYR | 563 | 69.151 | -2.569 | 10.562 | 1.00 | 36.17 |
| ATOM | 4356 | N | ALA | 564 | 67.711 | -1.234 | 9.454 | 1.00 | 39.60 |
| ATOM | 4358 | CA | ALA | 564 | 66.529 | -2.025 | 9.750 | 1.00 | 38.93 |
| ATOM | 4359 | CB | ALA | 564 | 65.557 | -1.207 | 10.570 | 1.00 | 40.23 |
| ATOM | 4360 | C | ALA | 564 | 65.919 | -2.360 | 8.394 | 1.00 | 41.61 |
| ATOM | 4361 | O | ALA | 564 | 64.958 | -1.736 | 7.977 | 1.00 | 45.88 |
| ATOM | 4362 | N | SER | 565 | 66.455 | -3.387 | 7.745 | 1.00 | 41.15 |
| ATOM | 4364 | CA | SER | 565 | 66.018 | -3.806 | 6.421 | 1.00 | 40.40 |
| ATOM | 4365 | CB | SER | 565 | 66.673 | -5.134 | 6.070 | 1.00 | 40.15 |
| ATOM | 4366 | OG | SER | 565 | 66.646 | -6.012 | 7.175 | 1.00 | 33.93 |
| ATOM | 4368 | C | SER | 565 | 64.530 | -3.932 | 6.164 | 1.00 | 40.31 |
| ATOM | 4369 | O | SER | 565 | 64.097 | -3.823 | 5.025 | 1.00 | 45.43 |
| ATOM | 4370 | N | LYS | 566 | 63.743 | -4.183 | 7.197 | 1.00 | 39.63 |
| ATOM | 4372 | CA | LYS | 566 | 62.312 | -4.341 | 6.992 | 1.00 | 38.01 |
| ATOM | 4373 | CB | LYS | 566 | 61.807 | -5.541 | 7.783 | 1.00 | 38.35 |
| ATOM | 4374 | CG | LYS | 566 | 62.468 | -6.828 | 7.308 | 1.00 | 38.21 |
| ATOM | 4375 | CD | LYS | 566 | 62.161 | -8.004 | 8.208 | 1.00 | 38.79 |
| ATOM | 4376 | CE | LYS | 566 | 62.734 | -9.277 | 7.621 | 1.00 | 38.76 |
| ATOM | 4377 | NZ | LYS | 566 | 62.692 | -10.400 | 8.598 | 1.00 | 42.40 |
| ATOM | 4381 | C | LYS | 566 | 61.488 | -3.079 | 7.249 | 1.00 | 37.28 |
| ATOM | 4382 | O | LYS | 566 | 60.265 | -3.132 | 7.415 | 1.00 | 39.48 |
| ATOM | 4383 | N | GLY | 567 | 62.166 | -1.936 | 7.237 | 1.00 | 34.31 |
| ATOM | 4385 | CA | GLY | 567 | 61.497 | -0.666 | 7.428 | 1.00 | 32.82 |
| ATOM | 4386 | C | GLY | 567 | 60.810 | -0.473 | 8.761 | 1.00 | 31.33 |
| ATOM | 4387 | O | GLY | 567 | 61.251 | -1.012 | 9.778 | 1.00 | 29.23 |
| ATOM | 4388 | N | ASN | 568 | 59.722 | 0.294 | 8.754 | 1.00 | 29.92 |
| ATOM | 4390 | CA | ASN | 568 | 58.999 | 0.569 | 9.974 | 1.00 | 31.05 |
| ATOM | 4391 | CB | ASN | 568 | 58.414 | 1.991 | 9.991 | 1.00 | 31.23 |
| ATOM | 4392 | CG | ASN | 568 | 57.201 | 2.157 | 9.087 | 1.00 | 34.16 |
| ATOM | 4393 | OD1 | ASN | 568 | 56.095 | 1.685 | 9.385 | 1.00 | 37.22 |
| ATOM | 4394 | ND2 | ASN | 568 | 57.394 | 2.877 | 7.999 | 1.00 | 35.13 |
| ATOM | 4397 | C | ASN | 568 | 57.950 | -0.486 | 10.235 | 1.00 | 31.60 |
| ATOM | 4398 | O | ASN | 568 | 57.535 | -1.205 | 9.324 | 1.00 | 31.76 |
| ATOM | 4399 | N | LEU | 569 | 57.517 | -0.548 | 11.490 | 1.00 | 34.63 |
| ATOM | 4401 | CA | LEU | 569 | 56.540 | -1.511 | 11.979 | 1.00 | 35.49 |
| ATOM | 4402 | CB | LEU | 569 | 56.456 | -1.408 | 13.500 | 1.00 | 36.13 |
| ATOM | 4403 | CG | LEU | 569 | 55.509 | -2.363 | 14.210 | 1.00 | 34.78 |
| ATOM | 4404 | CD1 | LEU | 569 | 56.010 | -3.804 | 14.034 | 1.00 | 35.01 |
| ATOM | 4405 | CD2 | LEU | 569 | 55.425 | -1.971 | 15.664 | 1.00 | 31.13 |
| ATOM | 4406 | C | LEU | 569 | 55.141 | -1.420 | 11.382 | 1.00 | 37.34 |
| ATOM | 4407 | O | LEU | 569 | 54.518 | -2.447 | 11.141 | 1.00 | 41.49 |
| ATOM | 4408 | N | ARG | 570 | 54.636 | -0.213 | 11.162 | 1.00 | 37.19 |
| ATOM | 4410 | CA | ARG | 570 | 53.299 | -0.063 | 10.591 | 1.00 | 39.79 |
| ATOM | 4411 | CB | ARG | 570 | 52.979 | 1.403 | 10.331 | 1.00 | 39.48 |
| ATOM | 4412 | CG | ARG | 570 | 51.558 | 1.638 | 9.887 | 1.00 | 41.93 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4413 | CD | ARG | 570 | 51.459 | 2.966 | 9.182 | 1.00 | 49.89 |
| ATOM | 4414 | NE | ARG | 570 | 52.329 | 2.991 | 8.009 | 1.00 | 55.25 |
| ATOM | 4416 | CZ | ARG | 570 | 53.121 | 4.008 | 7.693 | 1.00 | 57.90 |
| ATOM | 4417 | NH1 | ARG | 570 | 53.145 | 5.093 | 8.455 | 1.00 | 56.93 |
| ATOM | 4420 | NH2 | ARG | 570 | 53.921 | 3.920 | 6.637 | 1.00 | 57.58 |
| ATOM | 4423 | C | ARG | 570 | 53.219 | -0.835 | 9.278 | 1.00 | 39.84 |
| ATOM | 4424 | O | ARG | 570 | 52.309 | -1.644 | 9.060 | 1.00 | 42.48 |
| ATOM | 4425 | N | GLU | 571 | 54.208 | -0.597 | 8.425 | 1.00 | 38.22 |
| ATOM | 4427 | CA | GLU | 571 | 54.292 | -1.251 | 7.135 | 1.00 | 38.84 |
| ATOM | 4428 | CB | GLU | 571 | 55.284 | -0.492 | 6.266 | 1.00 | 40.72 |
| ATOM | 4429 | CG | GLU | 571 | 54.818 | 0.941 | 5.999 | 1.00 | 49.17 |
| ATOM | 4430 | CD | GLU | 571 | 55.845 | 1.798 | 5.284 | 1.00 | 58.95 |
| ATOM | 4431 | OE1 | GLU | 571 | 57.047 | 1.434 | 5.278 | 1.00 | 67.07 |
| ATOM | 4432 | OE2 | GLU | 571 | 55.455 | 2.854 | 4.736 | 1.00 | 61.02 |
| ATOM | 4433 | C | GLU | 571 | 54.617 | -2.744 | 7.240 | 1.00 | 37.79 |
| ATOM | 4434 | O | GLU | 571 | 54.075 | -3.558 | 6.488 | 1.00 | 37.63 |
| ATOM | 4435 | N | TYR | 572 | 55.462 | -3.104 | 8.204 | 1.00 | 36.89 |
| ATOM | 4437 | CA | TYR | 572 | 55.841 | -4.498 | 8.437 | 1.00 | 36.81 |
| ATOM | 4438 | CB | TYR | 572 | 56.822 | -4.584 | 9.612 | 1.00 | 33.24 |
| ATOM | 4439 | CG | TYR | 572 | 57.191 | -5.987 | 10.080 | 1.00 | 33.42 |
| ATOM | 4440 | CD1 | TYR | 572 | 58.209 | -6.714 | 9.450 | 1.00 | 31.93 |
| ATOM | 4441 | CE1 | TYR | 572 | 58.623 | -7.960 | 9.936 | 1.00 | 30.14 |
| ATOM | 4442 | CD2 | TYR | 572 | 56.586 | -6.552 | 11.208 | 1.00 | 34.42 |
| ATOM | 4443 | CE2 | TYR | 572 | 56.991 | -7.799 | 11.704 | 1.00 | 32.29 |
| ATOM | 4444 | CZ | TYR | 572 | 58.012 | -8.495 | 11.065 | 1.00 | 32.52 |
| ATOM | 4445 | OH | TYR | 572 | 58.427 | -9.717 | 11.571 | 1.00 | 31.70 |
| ATOM | 4447 | C | TYR | 572 | 54.588 | -5.310 | 8.754 | 1.00 | 37.64 |
| ATOM | 4448 | O | TYR | 572 | 54.387 | -6.410 | 8.226 | 1.00 | 35.70 |
| ATOM | 4449 | N | LEU | 573 | 53.742 | -4.740 | 9.608 | 1.00 | 38.63 |
| ATOM | 4451 | CA | LEU | 573 | 52.498 | -5.376 | 10.011 | 1.00 | 38.21 |
| ATOM | 4452 | CB | LEU | 573 | 51.802 | -4.532 | 11.067 | 1.00 | 35.40 |
| ATOM | 4453 | CG | LEU | 573 | 52.494 | -4.421 | 12.419 | 1.00 | 34.55 |
| ATOM | 4454 | CD1 | LEU | 573 | 51.755 | -3.402 | 13.258 | 1.00 | 32.02 |
| ATOM | 4455 | CD2 | LEU | 573 | 52.537 | -5.788 | 13.108 | 1.00 | 34.58 |
| ATOM | 4456 | C | LEU | 573 | 51.570 | -5.549 | 8.818 | 1.00 | 38.11 |
| ATOM | 4457 | O | LEU | 573 | 51.144 | -6.656 | 8.507 | 1.00 | 37.68 |
| ATOM | 4458 | N | GLN | 574 | 51.286 | -4.448 | 8.138 | 1.00 | 40.92 |
| ATOM | 4460 | CA | GLN | 574 | 50.402 | -4.476 | 6.982 | 1.00 | 45.16 |
| ATOM | 4461 | CB | GLN | 574 | 50.213 | -3.071 | 6.447 | 1.00 | 44.16 |
| ATOM | 4462 | CG | GLN | 574 | 49.380 | -2.239 | 7.369 | 1.00 | 45.26 |
| ATOM | 4463 | CD | GLN | 574 | 49.222 | -0.849 | 6.863 | 1.00 | 47.09 |
| ATOM | 4464 | OE1 | GLN | 574 | 49.789 | -0.483 | 5.838 | 1.00 | 50.83 |
| ATOM | 4465 | NE2 | GLN | 574 | 48.450 | -0.051 | 7.573 | 1.00 | 48.95 |
| ATOM | 4468 | C | GLN | 574 | 50.807 | -5.419 | 5.861 | 1.00 | 45.21 |
| ATOM | 4469 | O | GLN | 574 | 49.951 | -6.031 | 5.215 | 1.00 | 49.63 |
| ATOM | 4470 | N | ALA | 575 | 52.105 | -5.562 | 5.646 | 1.00 | 43.35 |
| ATOM | 4472 | CA | ALA | 575 | 52.579 | -6.446 | 4.604 | 1.00 | 42.62 |
| ATOM | 4473 | CB | ALA | 575 | 54.023 | -6.130 | 4.284 | 1.00 | 43.49 |
| ATOM | 4474 | C | ALA | 575 | 52.439 | -7.906 | 5.022 | 1.00 | 42.85 |
| ATOM | 4475 | O | ALA | 575 | 52.771 | -8.804 | 4.254 | 1.00 | 44.43 |
| ATOM | 4476 | N | ARG | 576 | 51.937 | -8.142 | 6.229 | 1.00 | 42.24 |
| ATOM | 4478 | CA | ARG | 576 | 51.787 | -9.494 | 6.747 | 1.00 | 41.58 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4479 | CB | ARG | 576 | 52.813 | -9.725 | 7.849 | 1.00 | 40.10 |
| ATOM | 4480 | CG | ARG | 576 | 54.225 | -9.694 | 7.314 | 1.00 | 40.58 |
| ATOM | 4481 | CD | ARG | 576 | 55.280 | -9.604 | 8.392 | 1.00 | 42.40 |
| ATOM | 4482 | NE | ARG | 576 | 56.632 | -9.607 | 7.826 | 1.00 | 41.95 |
| ATOM | 4484 | CZ | ARG | 576 | 57.110 | -8.684 | 6.992 | 1.00 | 38.22 |
| ATOM | 4485 | NH1 | ARG | 576 | 56.359 | -7.658 | 6.612 | 1.00 | 38.61 |
| ATOM | 4488 | NH2 | ARG | 576 | 58.347 | -8.787 | 6.541 | 1.00 | 34.50 |
| ATOM | 4491 | C | ARG | 576 | 50.389 | -9.762 | 7.255 | 1.00 | 43.28 |
| ATOM | 4492 | O | ARG | 576 | 50.187 | -10.607 | 8.137 | 1.00 | 43.76 |
| ATOM | 4493 | N | ARG | 577 | 49.418 | -9.057 | 6.684 | 1.00 | 44.65 |
| ATOM | 4495 | CA | ARG | 577 | 48.023 | -9.222 | 7.077 | 1.00 | 46.69 |
| ATOM | 4496 | CB | ARG | 577 | 47.197 | -8.032 | 6.587 | 1.00 | 45.24 |
| ATOM | 4497 | CG | ARG | 577 | 47.372 | -6.793 | 7.440 | 1.00 | 42.93 |
| ATOM | 4498 | CD | ARG | 577 | 46.572 | -5.635 | 6.898 | 1.00 | 44.63 |
| ATOM | 4499 | NE | ARG | 577 | 46.428 | -4.577 | 7.895 | 1.00 | 47.76 |
| ATOM | 4501 | CZ | ARG | 577 | 45.750 | -3.450 | 7.704 | 1.00 | 48.55 |
| ATOM | 4502 | NH1 | ARG | 577 | 45.149 | -3.225 | 6.548 | 1.00 | 50.64 |
| ATOM | 4505 | NH2 | ARG | 577 | 45.643 | -2.560 | 8.684 | 1.00 | 50.77 |
| ATOM | 4508 | C | ARG | 577 | 47.408 | -10.540 | 6.603 | 1.00 | 47.12 |
| ATOM | 4509 | O | ARG | 577 | 47.396 | -10.840 | 5.406 | 1.00 | 48.37 |
| ATOM | 4510 | N | GLN | 594 | 53.246 | -13.695 | 7.891 | 1.00 | 64.66 |
| ATOM | 4512 | CA | GLN | 594 | 52.054 | -13.835 | 8.728 | 1.00 | 65.10 |
| ATOM | 4513 | CB | GLN | 594 | 51.130 | -14.931 | 8.184 | 1.00 | 65.77 |
| ATOM | 4514 | C | GLN | 594 | 52.447 | -14.127 | 10.174 | 1.00 | 64.01 |
| ATOM | 4515 | O | GLN | 594 | 52.962 | -15.201 | 10.507 | 1.00 | 64.42 |
| ATOM | 4516 | N | LEU | 595 | 52.189 | -13.154 | 11.031 | 1.00 | 61.45 |
| ATOM | 4518 | CA | LEU | 595 | 52.524 | -13.245 | 12.437 | 1.00 | 59.21 |
| ATOM | 4519 | CB | LEU | 595 | 52.669 | -11.826 | 12.979 | 1.00 | 57.54 |
| ATOM | 4520 | CG | LEU | 595 | 53.648 | -11.043 | 12.099 | 1.00 | 56.37 |
| ATOM | 4521 | CD1 | LEU | 595 | 53.442 | -9.551 | 12.202 | 1.00 | 57.06 |
| ATOM | 4522 | CD2 | LEU | 595 | 55.064 | -11.430 | 12.465 | 1.00 | 55.57 |
| ATOM | 4523 | C | LEU | 595 | 51.509 | -14.046 | 13.257 | 1.00 | 58.34 |
| ATOM | 4524 | O | LEU | 595 | 50.316 | -14.039 | 12.953 | 1.00 | 58.21 |
| ATOM | 4525 | N | SER | 596 | 52.007 | -14.740 | 14.280 | 1.00 | 58.00 |
| ATOM | 4527 | CA | SER | 596 | 51.182 | -15.543 | 15.180 | 1.00 | 56.04 |
| ATOM | 4528 | CB | SER | 596 | 51.960 | -16.770 | 15.667 | 1.00 | 57.98 |
| ATOM | 4529 | OG | SER | 596 | 52.987 | -16.403 | 16.580 | 1.00 | 58.94 |
| ATOM | 4531 | C | SER | 596 | 50.854 | -14.681 | 16.383 | 1.00 | 54.65 |
| ATOM | 4532 | O | SER | 596 | 51.479 | -13.645 | 16.584 | 1.00 | 52.05 |
| ATOM | 4533 | N | SER | 597 | 49.914 | -15.133 | 17.208 | 1.00 | 56.10 |
| ATOM | 4535 | CA | SER | 597 | 49.525 | -14.389 | 18.398 | 1.00 | 57.51 |
| ATOM | 4536 | CB | SER | 597 | 48.530 | -15.196 | 19.236 | 1.00 | 58.60 |
| ATOM | 4537 | OG | SER | 597 | 47.620 | -15.914 | 18.421 | 1.00 | 61.95 |
| ATOM | 4539 | C | SER | 597 | 50.778 | -14.094 | 19.220 | 1.00 | 57.75 |
| ATOM | 4540 | O | SER | 597 | 50.934 | -12.998 | 19.755 | 1.00 | 57.86 |
| ATOM | 4541 | N | LYS | 598 | 51.692 | -15.062 | 19.271 | 1.00 | 57.88 |
| ATOM | 4543 | CA | LYS | 598 | 52.930 | -14.905 | 20.026 | 1.00 | 57.51 |
| ATOM | 4544 | CB | LYS | 598 | 53.690 | -16.231 | 20.124 | 1.00 | 57.72 |
| ATOM | 4545 | CG | LYS | 598 | 54.470 | -16.395 | 21.432 | 1.00 | 60.14 |
| ATOM | 4546 | CD | LYS | 598 | 55.227 | -17.724 | 21.479 | 1.00 | 62.23 |
| ATOM | 4547 | CE | LYS | 598 | 55.894 | -17.989 | 22.834 | 1.00 | 60.79 |
| ATOM | 4548 | NZ | LYS | 598 | 54.921 | -18.149 | 23.949 | 1.00 | 61.46 |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4552 | C | LYS | 598 | 53.809 | -13.829 | 19.389 | 1.00 | 55.94 | |
| ATOM | 4553 | O | LYS | 598 | 54.322 | -12.955 | 20.089 | 1.00 | 55.84 | |
| ATOM | 4554 | N | ASP | 599 | 53.935 | -13.866 | 18.061 | 1.00 | 53.32 | |
| ATOM | 4556 | CA | ASP | 599 | 54.737 | -12.882 | 17.334 | 1.00 | 50.30 | |
| ATOM | 4557 | CB | ASP | 599 | 54.688 | -13.119 | 15.823 | 1.00 | 49.72 | |
| ATOM | 4558 | CG | ASP | 599 | 55.426 | -14.383 | 15.394 | 1.00 | 53.97 | |
| ATOM | 4559 | OD1 | ASP | 599 | 56.176 | -14.948 | 16.214 | 1.00 | 58.12 | |
| ATOM | 4560 | OD2 | ASP | 599 | 55.261 | -14.822 | 14.233 | 1.00 | 55.58 | |
| ATOM | 4561 | C | ASP | 599 | 54.247 | -11.474 | 17.636 | 1.00 | 49.53 | |
| ATOM | 4562 | O | ASP | 599 | 55.054 | -10.589 | 17.911 | 1.00 | 51.16 | |
| ATOM | 4563 | N | LEU | 600 | 52.930 | -11.281 | 17.634 | 1.00 | 47.50 | |
| ATOM | 4565 | CA | LEU | 600 | 52.354 | -9.972 | 17.909 | 1.00 | 45.41 | |
| ATOM | 4566 | CB | LEU | 600 | 50.850 | -9.948 | 17.627 | 1.00 | 43.77 | |
| ATOM | 4567 | CG | LEU | 600 | 50.429 | -10.121 | 16.169 | 1.00 | 41.05 | |
| ATOM | 4568 | CD1 | LEU | 600 | 48.941 | -9.904 | 16.048 | 1.00 | 41.04 | |
| ATOM | 4569 | CD2 | LEU | 600 | 51.160 | -9.140 | 15.294 | 1.00 | 39.59 | |
| ATOM | 4570 | C | LEU | 600 | 52.638 | -9.485 | 19.318 | 1.00 | 46.77 | |
| ATOM | 4571 | O | LEU | 600 | 52.964 | -8.308 | 19.497 | 1.00 | 48.74 | |
| ATOM | 4572 | N | VAL | 601 | 52.524 | -10.372 | 20.314 | 1.00 | 47.64 | |
| ATOM | 4574 | CA | VAL | 601 | 52.804 | -10.002 | 21.716 | 1.00 | 47.38 | |
| ATOM | 4575 | CB | VAL | 601 | 52.321 | -11.070 | 22.756 | 1.00 | 46.58 | |
| ATOM | 4576 | CG1 | VAL | 601 | 52.081 | -10.403 | 24.114 | 1.00 | 45.07 | |
| ATOM | 4577 | CG2 | VAL | 601 | 51.058 | -11.759 | 22.306 | 1.00 | 48.86 | |
| ATOM | 4578 | C | VAL | 601 | 54.321 | -9.811 | 21.890 | 1.00 | 46.04 | |
| ATOM | 4579 | O | VAL | 601 | 54.793 | -8.935 | 22.622 | 1.00 | 46.13 | |
| ATOM | 4580 | N | SER | 602 | 55.090 | -10.624 | 21.183 | 1.00 | 44.21 | |
| ATOM | 4582 | CA | SER | 602 | 56.534 | -10.546 | 21.233 | 1.00 | 42.78 | |
| ATOM | 4583 | CB | SER | 602 | 57.119 | -11.594 | 20.297 | 1.00 | 43.98 | |
| ATOM | 4584 | OG | SER | 602 | 58.523 | -11.615 | 20.355 | 1.00 | 51.02 | |
| ATOM | 4586 | C | SER | 602 | 56.954 | -9.135 | 20.813 | 1.00 | 41.74 | |
| ATOM | 4587 | O | SER | 602 | 57.709 | -8.467 | 21.524 | 1.00 | 44.09 | |
| ATOM | 4588 | N | CYS | 603 | 56.425 | -8.667 | 19.685 | 1.00 | 39.57 | |
| ATOM | 4590 | CA | CYS | 603 | 56.699 | -7.317 | 19.177 | 1.00 | 36.11 | |
| ATOM | 4591 | CB | CYS | 603 | 55.852 | -7.058 | 17.924 | 1.00 | 34.72 | |
| ATOM | 4592 | SG | CYS | 603 | 55.760 | -5.364 | 17.323 | 0.50 | 29.10 | PRT1 |
| ATOM | 4593 | C | CYS | 603 | 56.378 | -6.272 | 20.252 | 1.00 | 34.50 | |
| ATOM | 4594 | O | CYS | 603 | 57.174 | -5.371 | 20.506 | 1.00 | 33.61 | |
| ATOM | 4595 | N | ALA | 604 | 55.236 | -6.429 | 20.913 | 1.00 | 34.64 | |
| ATOM | 4597 | CA | ALA | 604 | 54.811 | -5.506 | 21.964 | 1.00 | 37.18 | |
| ATOM | 4598 | CB | ALA | 604 | 53.386 | -5.850 | 22.414 | 1.00 | 38.20 | |
| ATOM | 4599 | C | ALA | 604 | 55.786 | -5.516 | 23.160 | 1.00 | 38.91 | |
| ATOM | 4600 | O | ALA | 604 | 56.026 | -4.481 | 23.790 | 1.00 | 38.29 | |
| ATOM | 4601 | N | TYR | 605 | 56.323 | -6.693 | 23.477 | 1.00 | 39.54 | |
| ATOM | 4603 | CA | TYR | 605 | 57.283 | -6.854 | 24.565 | 1.00 | 39.29 | |
| ATOM | 4604 | CB | TYR | 605 | 57.573 | -8.340 | 24.791 | 1.00 | 40.07 | |
| ATOM | 4605 | CG | TYR | 605 | 58.663 | -8.622 | 25.807 | 1.00 | 39.09 | |
| ATOM | 4606 | CD1 | TYR | 605 | 58.525 | -8.236 | 27.137 | 1.00 | 38.50 | |
| ATOM | 4607 | CE1 | TYR | 605 | 59.526 | -8.505 | 28.074 | 1.00 | 40.76 | |
| ATOM | 4608 | CD2 | TYR | 605 | 59.831 | -9.283 | 25.435 | 1.00 | 39.73 | |
| ATOM | 4609 | CE2 | TYR | 605 | 60.834 | -9.553 | 26.361 | 1.00 | 37.45 | |
| ATOM | 4610 | CZ | TYR | 605 | 60.678 | -9.166 | 27.677 | 1.00 | 40.34 | |
| ATOM | 4611 | OH | TYR | 605 | 61.666 | -9.466 | 28.601 | 1.00 | 43.16 | |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4613 | C | TYR | 605 | 58.582 | -6.113 | 24.224 | 1.00 | 39.45 |
| ATOM | 4614 | O | TYR | 605 | 59.067 | -5.291 | 25.022 | 1.00 | 38.75 |
| ATOM | 4615 | N | GLN | 606 | 59.129 | -6.410 | 23.040 | 1.00 | 36.41 |
| ATOM | 4617 | CA | GLN | 606 | 60.361 | -5.787 | 22.550 | 1.00 | 35.20 |
| ATOM | 4618 | CB | GLN | 606 | 60.695 | -6.303 | 21.150 | 1.00 | 34.86 |
| ATOM | 4619 | CG | GLN | 606 | 61.286 | -7.695 | 21.118 | 1.00 | 32.21 |
| ATOM | 4620 | CD | GLN | 606 | 61.502 | -8.205 | 19.709 | 1.00 | 32.63 |
| ATOM | 4621 | OE1 | GLN | 606 | 62.495 | -7.888 | 19.075 | 1.00 | 32.16 |
| ATOM | 4622 | NE2 | GLN | 606 | 60.568 | -9.004 | 19.216 | 1.00 | 34.62 |
| ATOM | 4625 | C | GLN | 606 | 60.286 | -4.252 | 22.525 | 1.00 | 36.03 |
| ATOM | 4626 | O | GLN | 606 | 61.209 | -3.572 | 22.989 | 1.00 | 38.81 |
| ATOM | 4627 | N | VAL | 607 | 59.188 | -3.716 | 21.998 | 1.00 | 33.45 |
| ATOM | 4629 | CA | VAL | 607 | 58.979 | -2.280 | 21.923 | 1.00 | 29.34 |
| ATOM | 4630 | CB | VAL | 607 | 57.651 | -1.948 | 21.189 | 1.00 | 28.80 |
| ATOM | 4631 | CG1 | VAL | 607 | 57.260 | -0.495 | 21.401 | 1.00 | 26.68 |
| ATOM | 4632 | CG2 | VAL | 607 | 57.790 | -2.244 | 19.699 | 1.00 | 24.66 |
| ATOM | 4633 | C | VAL | 607 | 58.965 | -1.698 | 23.339 | 1.00 | 31.35 |
| ATOM | 4634 | O | VAL | 607 | 59.557 | -0.643 | 23.579 | 1.00 | 33.86 |
| ATOM | 4635 | N | ALA | 608 | 58.317 | -2.402 | 24.270 | 1.00 | 30.17 |
| ATOM | 4637 | CA | ALA | 608 | 58.235 | -1.971 | 25.667 | 1.00 | 28.98 |
| ATOM | 4638 | CB | ALA | 608 | 57.255 | -2.836 | 26.440 | 1.00 | 28.30 |
| ATOM | 4639 | C | ALA | 608 | 59.598 | -1.979 | 26.352 | 1.00 | 28.94 |
| ATOM | 4640 | O | ALA | 608 | 59.889 | -1.091 | 27.155 | 1.00 | 27.83 |
| ATOM | 4641 | N | ARG | 609 | 60.436 | -2.959 | 26.032 | 1.00 | 28.79 |
| ATOM | 4643 | CA | ARG | 609 | 61.765 | -3.023 | 26.628 | 1.00 | 30.90 |
| ATOM | 4644 | CB | ARG | 609 | 62.499 | -4.291 | 26.206 | 1.00 | 35.84 |
| ATOM | 4645 | CG | ARG | 609 | 61.787 | -5.571 | 26.527 | 1.00 | 41.94 |
| ATOM | 4646 | CD | ARG | 609 | 62.782 | -6.707 | 26.575 | 1.00 | 44.70 |
| ATOM | 4647 | NE | ARG | 609 | 63.392 | -6.821 | 27.900 | 1.00 | 47.13 |
| ATOM | 4649 | CZ | ARG | 609 | 64.444 | -7.589 | 28.183 | 1.00 | 48.71 |
| ATOM | 4650 | NH1 | ARG | 609 | 65.025 | -8.314 | 27.233 | 1.00 | 48.33 |
| ATOM | 4653 | NH2 | ARG | 609 | 64.897 | -7.655 | 29.428 | 1.00 | 49.11 |
| ATOM | 4656 | C | ARG | 609 | 62.602 | -1.815 | 26.207 | 1.00 | 32.38 |
| ATOM | 4657 | O | ARG | 609 | 63.215 | -1.148 | 27.058 | 1.00 | 32.63 |
| ATOM | 4658 | N | GLY | 610 | 62.636 | -1.554 | 24.894 | 1.00 | 29.98 |
| ATOM | 4660 | CA | GLY | 610 | 63.384 | -0.430 | 24.358 | 1.00 | 25.65 |
| ATOM | 4661 | C | GLY | 610 | 62.969 | 0.837 | 25.061 | 1.00 | 25.44 |
| ATOM | 4662 | O | GLY | 610 | 63.791 | 1.640 | 25.463 | 1.00 | 27.09 |
| ATOM | 4663 | N | MET | 611 | 61.672 | 1.009 | 25.242 | 1.00 | 30.41 |
| ATOM | 4665 | CA | MET | 611 | 61.167 | 2.176 | 25.943 | 1.00 | 31.34 |
| ATOM | 4666 | CB | MET | 611 | 59.653 | 2.233 | 25.832 | 1.00 | 28.39 |
| ATOM | 4667 | CG | MET | 611 | 59.195 | 2.595 | 24.449 | 1.00 | 25.17 |
| ATOM | 4668 | SD | MET | 611 | 59.904 | 4.182 | 24.005 | 1.00 | 26.65 |
| ATOM | 4669 | CE | MET | 611 | 59.458 | 5.158 | 25.453 | 1.00 | 19.78 |
| ATOM | 4670 | C | MET | 611 | 61.600 | 2.176 | 27.412 | 1.00 | 34.05 |
| ATOM | 4671 | O | MET | 611 | 62.008 | 3.211 | 27.929 | 1.00 | 33.79 |
| ATOM | 4672 | N | GLU | 612 | 61.500 | 1.026 | 28.078 | 1.00 | 37.16 |
| ATOM | 4674 | CA | GLU | 612 | 61.893 | 0.913 | 29.484 | 1.00 | 38.85 |
| ATOM | 4675 | CB | GLU | 612 | 61.732 | -0.533 | 29.988 | 1.00 | 38.96 |
| ATOM | 4676 | CG | GLU | 612 | 62.249 | -0.788 | 31.400 | 1.00 | 35.19 |
| ATOM | 4677 | CD | GLU | 612 | 62.316 | -2.271 | 31.783 | 1.00 | 35.26 |
| ATOM | 4678 | OE1 | GLU | 612 | 62.605 | -3.123 | 30.912 | 1.00 | 29.29 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4679 | OE2 | GLU | 612 | 62.102 | -2.588 | 32.982 | 1.00 | 37.85 |
| ATOM | 4680 | C | GLU | 612 | 63.353 | 1.364 | 29.628 | 1.00 | 40.01 |
| ATOM | 4681 | O | GLU | 612 | 63.720 | 2.060 | 30.584 | 1.00 | 38.27 |
| ATOM | 4682 | N | TYR | 613 | 64.176 | 0.972 | 28.662 | 1.00 | 40.33 |
| ATOM | 4684 | CA | TYR | 613 | 65.575 | 1.362 | 28.664 | 1.00 | 39.71 |
| ATOM | 4685 | CB | TYR | 613 | 66.333 | 0.722 | 27.494 | 1.00 | 39.03 |
| ATOM | 4686 | CG | TYR | 613 | 67.800 | 1.100 | 27.467 | 1.00 | 41.41 |
| ATOM | 4687 | CD1 | TYR | 613 | 68.702 | 0.527 | 28.364 | 1.00 | 42.79 |
| ATOM | 4688 | CE1 | TYR | 613 | 70.048 | 0.905 | 28.386 | 1.00 | 40.21 |
| ATOM | 4689 | CD2 | TYR | 613 | 68.283 | 2.068 | 26.581 | 1.00 | 39.75 |
| ATOM | 4690 | CE2 | TYR | 613 | 69.621 | 2.454 | 26.596 | 1.00 | 39.01 |
| ATOM | 4691 | CZ | TYR | 613 | 70.499 | 1.868 | 27.503 | 1.00 | 39.56 |
| ATOM | 4692 | OH | TYR | 613 | 71.823 | 2.249 | 27.538 | 1.00 | 35.63 |
| ATOM | 4694 | C | TYR | 613 | 65.642 | 2.881 | 28.562 | 1.00 | 38.71 |
| ATOM | 4695 | O | TYR | 613 | 66.106 | 3.541 | 29.486 | 1.00 | 38.52 |
| ATOM | 4696 | N | LEU | 614 | 65.126 | 3.423 | 27.460 | 1.00 | 37.22 |
| ATOM | 4698 | CA | LEU | 614 | 65.128 | 4.864 | 27.212 | 1.00 | 35.66 |
| ATOM | 4699 | CB | LEU | 614 | 64.223 | 5.202 | 26.025 | 1.00 | 35.27 |
| ATOM | 4700 | CG | LEU | 614 | 64.687 | 4.699 | 24.659 | 1.00 | 33.09 |
| ATOM | 4701 | CD1 | LEU | 614 | 63.718 | 5.188 | 23.612 | 1.00 | 33.31 |
| ATOM | 4702 | CD2 | LEU | 614 | 66.099 | 5.184 | 24.363 | 1.00 | 31.20 |
| ATOM | 4703 | C | LEU | 614 | 64.672 | 5.653 | 28.430 | 1.00 | 35.64 |
| ATOM | 4704 | O | LEU | 614 | 65.298 | 6.639 | 28.816 | 1.00 | 34.54 |
| ATOM | 4705 | N | ALA | 615 | 63.577 | 5.203 | 29.032 | 1.00 | 36.61 |
| ATOM | 4707 | CA | ALA | 615 | 63.028 | 5.835 | 30.222 | 1.00 | 37.74 |
| ATOM | 4708 | CB | ALA | 615 | 61.682 | 5.187 | 30.608 | 1.00 | 37.74 |
| ATOM | 4709 | C | ALA | 615 | 64.021 | 5.776 | 31.389 | 1.00 | 37.30 |
| ATOM | 4710 | O | ALA | 615 | 64.111 | 6.731 | 32.175 | 1.00 | 37.29 |
| ATOM | 4711 | N | SER | 616 | 64.752 | 4.665 | 31.511 | 1.00 | 37.18 |
| ATOM | 4713 | CA | SER | 616 | 65.741 | 4.534 | 32.577 | 1.00 | 36.92 |
| ATOM | 4714 | CB | SER | 616 | 66.274 | 3.091 | 32.702 | 1.00 | 34.82 |
| ATOM | 4715 | OG | SER | 616 | 67.106 | 2.680 | 31.628 | 1.00 | 28.79 |
| ATOM | 4717 | C | SER | 616 | 66.870 | 5.516 | 32.287 | 1.00 | 38.57 |
| ATOM | 4718 | O | SER | 616 | 67.633 | 5.902 | 33.179 | 1.00 | 38.30 |
| ATOM | 4719 | N | LYS | 617 | 66.958 | 5.925 | 31.024 | 1.00 | 37.62 |
| ATOM | 4721 | CA | LYS | 617 | 67.965 | 6.876 | 30.606 | 1.00 | 36.13 |
| ATOM | 4722 | CB | LYS | 617 | 68.511 | 6.494 | 29.238 | 1.00 | 35.90 |
| ATOM | 4723 | CG | LYS | 617 | 69.274 | 5.206 | 29.236 | 1.00 | 34.58 |
| ATOM | 4724 | CD | LYS | 617 | 70.502 | 5.348 | 30.077 | 1.00 | 35.44 |
| ATOM | 4725 | CE | LYS | 617 | 71.201 | 4.022 | 30.232 | 1.00 | 38.54 |
| ATOM | 4726 | NZ | LYS | 617 | 72.566 | 4.211 | 30.790 | 1.00 | 41.54 |
| ATOM | 4730 | C | LYS | 617 | 67.378 | 8.275 | 30.564 | 1.00 | 36.55 |
| ATOM | 4731 | O | LYS | 617 | 67.943 | 9.155 | 29.934 | 1.00 | 40.26 |
| ATOM | 4732 | N | LYS | 618 | 66.221 | 8.468 | 31.187 | 1.00 | 36.42 |
| ATOM | 4734 | CA | LYS | 618 | 65.570 | 9.779 | 31.231 | 1.00 | 36.06 |
| ATOM | 4735 | CB | LYS | 618 | 66.543 | 10.833 | 31.746 | 1.00 | 42.22 |
| ATOM | 4736 | CG | LYS | 618 | 67.234 | 10.499 | 33.062 | 1.00 | 52.36 |
| ATOM | 4737 | CD | LYS | 618 | 66.301 | 10.668 | 34.236 | 1.00 | 61.51 |
| ATOM | 4738 | CE | LYS | 618 | 66.933 | 10.121 | 35.495 | 1.00 | 67.28 |
| ATOM | 4739 | NZ | LYS | 618 | 65.965 | 10.161 | 36.618 | 1.00 | 73.99 |
| ATOM | 4743 | C | LYS | 618 | 65.026 | 10.261 | 29.887 | 1.00 | 34.94 |
| ATOM | 4744 | O | LYS | 618 | 64.562 | 11.393 | 29.781 | 1.00 | 34.69 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4745 | N | CYS | 619 | 65.051 | 9.407 | 28.872 | 1.00 | 34.46 |
| ATOM | 4747 | CA | CYS | 619 | 64.588 | 9.793 | 27.543 | 1.00 | 33.12 |
| ATOM | 4748 | CB | CYS | 619 | 65.311 | 8.966 | 26.475 | 1.00 | 34.33 |
| ATOM | 4749 | SG | CYS | 619 | 64.920 | 9.397 | 24.778 | 1.00 | 35.64 |
| ATOM | 4750 | C | CYS | 619 | 63.075 | 9.699 | 27.355 | 1.00 | 32.13 |
| ATOM | 4751 | O | CYS | 619 | 62.465 | 8.645 | 27.584 | 1.00 | 30.72 |
| ATOM | 4752 | N | ILE | 620 | 62.477 | 10.818 | 26.960 | 1.00 | 32.70 |
| ATOM | 4754 | CA | ILE | 620 | 61.046 | 10.909 | 26.708 | 1.00 | 32.75 |
| ATOM | 4755 | CB | ILE | 620 | 60.440 | 12.129 | 27.421 | 1.00 | 33.55 |
| ATOM | 4756 | CG2 | ILE | 620 | 59.002 | 12.339 | 26.986 | 1.00 | 38.39 |
| ATOM | 4757 | CG1 | ILE | 620 | 60.486 | 11.913 | 28.933 | 1.00 | 30.71 |
| ATOM | 4758 | CD1 | ILE | 620 | 59.994 | 13.084 | 29.710 | 1.00 | 30.11 |
| ATOM | 4759 | C | ILE | 620 | 60.969 | 11.086 | 25.206 | 1.00 | 33.31 |
| ATOM | 4760 | O | ILE | 620 | 61.516 | 12.040 | 24.674 | 1.00 | 33.40 |
| ATOM | 4761 | N | HIS | 621 | 60.356 | 10.114 | 24.533 | 1.00 | 33.56 |
| ATOM | 4763 | CA | HIS | 621 | 60.230 | 10.092 | 23.087 | 1.00 | 32.30 |
| ATOM | 4764 | CB | HIS | 621 | 59.866 | 8.668 | 22.642 | 1.00 | 29.55 |
| ATOM | 4765 | CG | HIS | 621 | 60.049 | 8.402 | 21.173 | 1.00 | 27.32 |
| ATOM | 4766 | CD2 | HIS | 621 | 60.694 | 7.404 | 20.533 | 1.00 | 24.26 |
| ATOM | 4767 | ND1 | HIS | 621 | 59.462 | 9.173 | 20.187 | 1.00 | 25.20 |
| ATOM | 4769 | CE1 | HIS | 621 | 59.734 | 8.652 | 19.006 | 1.00 | 25.81 |
| ATOM | 4770 | NE2 | HIS | 621 | 60.481 | 7.579 | 19.184 | 1.00 | 26.65 |
| ATOM | 4772 | C | HIS | 621 | 59.246 | 11.103 | 22.499 | 1.00 | 35.40 |
| ATOM | 4773 | O | HIS | 621 | 59.459 | 11.574 | 21.388 | 1.00 | 39.18 |
| ATOM | 4774 | N | ARG | 622 | 58.128 | 11.363 | 23.178 | 1.00 | 36.39 |
| ATOM | 4776 | CA | ARG | 622 | 57.117 | 12.323 | 22.686 | 1.00 | 36.40 |
| ATOM | 4777 | CB | ARG | 622 | 57.694 | 13.732 | 22.617 | 1.00 | 35.62 |
| ATOM | 4778 | CG | ARG | 622 | 58.171 | 14.253 | 23.937 | 1.00 | 33.79 |
| ATOM | 4779 | CD | ARG | 622 | 58.837 | 15.591 | 23.759 | 0.50 | 32.17 |
| ATOM | 4780 | NE | ARG | 622 | 59.315 | 16.101 | 25.032 | 0.50 | 32.82 |
| ATOM | 4782 | CZ | ARG | 622 | 60.487 | 15.786 | 25.575 | 0.50 | 34.07 |
| ATOM | 4783 | NH1 | ARG | 622 | 61.326 | 14.965 | 24.952 | 0.50 | 33.44 |
| ATOM | 4786 | NH2 | ARG | 622 | 60.803 | 16.268 | 26.769 | 0.50 | 32.70 |
| ATOM | 4789 | C | ARG | 622 | 56.405 | 12.008 | 21.355 | 1.00 | 36.23 |
| ATOM | 4790 | O | ARG | 622 | 55.527 | 12.763 | 20.936 | 1.00 | 35.04 |
| ATOM | 4791 | N | ASP | 623 | 56.806 | 10.938 | 20.668 | 1.00 | 35.84 |
| ATOM | 4793 | CA | ASP | 623 | 56.128 | 10.538 | 19.436 | 1.00 | 35.68 |
| ATOM | 4794 | CB | ASP | 623 | 56.574 | 11.352 | 18.221 | 1.00 | 38.71 |
| ATOM | 4795 | CG | ASP | 623 | 55.736 | 11.036 | 16.974 | 1.00 | 46.29 |
| ATOM | 4796 | OD1 | ASP | 623 | 56.277 | 11.082 | 15.851 | 1.00 | 52.33 |
| ATOM | 4797 | OD2 | ASP | 623 | 54.535 | 10.715 | 17.119 | 1.00 | 50.45 |
| ATOM | 4798 | C | ASP | 623 | 56.271 | 9.052 | 19.162 | 1.00 | 32.98 |
| ATOM | 4799 | O | ASP | 623 | 56.664 | 8.645 | 18.073 | 1.00 | 30.90 |
| ATOM | 4800 | N | LEU | 624 | 56.015 | 8.244 | 20.179 | 1.00 | 31.16 |
| ATOM | 4802 | CA | LEU | 624 | 56.099 | 6.801 | 20.029 | 1.00 | 31.71 |
| ATOM | 4803 | CB | LEU | 624 | 56.070 | 6.144 | 21.407 | 1.00 | 28.48 |
| ATOM | 4804 | CG | LEU | 624 | 56.049 | 4.618 | 21.514 | 1.00 | 28.13 |
| ATOM | 4805 | CD1 | LEU | 624 | 57.225 | 3.975 | 20.799 | 1.00 | 27.00 |
| ATOM | 4806 | CD2 | LEU | 624 | 56.072 | 4.283 | 22.987 | 1.00 | 29.10 |
| ATOM | 4807 | C | LEU | 624 | 54.917 | 6.320 | 19.185 | 1.00 | 32.67 |
| ATOM | 4808 | O | LEU | 624 | 53.763 | 6.608 | 19.508 | 1.00 | 35.74 |
| ATOM | 4809 | N | ALA | 625 | 55.214 | 5.640 | 18.081 | 1.00 | 29.82 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4811 | CA | ALA | 625 | 54.194 | 5.106 | 17.181 | 1.00 | 28.29 |
| ATOM | 4812 | CB | ALA | 625 | 53.682 | 6.182 | 16.245 | 1.00 | 26.72 |
| ATOM | 4813 | C | ALA | 625 | 54.895 | 4.031 | 16.395 | 1.00 | 28.40 |
| ATOM | 4814 | O | ALA | 625 | 56.118 | 4.028 | 16.343 | 1.00 | 32.12 |
| ATOM | 4815 | N | ALA | 626 | 54.131 | 3.135 | 15.770 | 1.00 | 28.55 |
| ATOM | 4817 | CA | ALA | 626 | 54.687 | 2.028 | 14.979 | 1.00 | 26.25 |
| ATOM | 4818 | CB | ALA | 626 | 53.577 | 1.169 | 14.365 | 1.00 | 23.54 |
| ATOM | 4819 | C | ALA | 626 | 55.569 | 2.573 | 13.892 | 1.00 | 23.68 |
| ATOM | 4820 | O | ALA | 626 | 56.544 | 1.944 | 13.519 | 1.00 | 26.07 |
| ATOM | 4821 | N | ARG | 627 | 55.208 | 3.744 | 13.378 | 1.00 | 23.80 |
| ATOM | 4823 | CA | ARG | 627 | 55.980 | 4.413 | 12.338 | 1.00 | 26.57 |
| ATOM | 4824 | CB | ARG | 627 | 55.289 | 5.728 | 11.914 | 1.00 | 25.91 |
| ATOM | 4825 | CG | ARG | 627 | 54.991 | 6.692 | 13.055 | 1.00 | 27.60 |
| ATOM | 4826 | CD | ARG | 627 | 54.711 | 8.130 | 12.584 | 1.00 | 33.01 |
| ATOM | 4827 | NE | ARG | 627 | 54.260 | 8.978 | 13.691 | 1.00 | 34.18 |
| ATOM | 4829 | CZ | ARG | 627 | 52.997 | 9.067 | 14.091 | 1.00 | 35.88 |
| ATOM | 4830 | NH1 | ARG | 627 | 52.056 | 8.380 | 13.460 | 1.00 | 38.89 |
| ATOM | 4833 | NH2 | ARG | 627 | 52.689 | 9.748 | 15.183 | 1.00 | 36.43 |
| ATOM | 4836 | C | ARG | 627 | 57.439 | 4.686 | 12.785 | 1.00 | 29.03 |
| ATOM | 4837 | O | ARG | 627 | 58.362 | 4.606 | 11.972 | 1.00 | 29.24 |
| ATOM | 4838 | N | ASN | 628 | 57.634 | 4.938 | 14.087 | 1.00 | 29.51 |
| ATOM | 4840 | CA | ASN | 628 | 58.954 | 5.234 | 14.645 | 1.00 | 26.41 |
| ATOM | 4841 | CB | ASN | 628 | 58.864 | 6.359 | 15.676 | 1.00 | 25.32 |
| ATOM | 4842 | CG | ASN | 628 | 58.539 | 7.687 | 15.035 | 1.00 | 28.11 |
| ATOM | 4843 | OD1 | ASN | 628 | 59.079 | 8.028 | 13.999 | 1.00 | 32.09 |
| ATOM | 4844 | ND2 | ASN | 628 | 57.639 | 8.426 | 15.628 | 1.00 | 27.88 |
| ATOM | 4847 | C | ASN | 628 | 59.684 | 4.039 | 15.225 | 1.00 | 25.77 |
| ATOM | 4848 | O | ASN | 628 | 60.641 | 4.188 | 16.001 | 1.00 | 24.77 |
| ATOM | 4849 | N | VAL | 629 | 59.209 | 2.853 | 14.874 | 1.00 | 26.63 |
| ATOM | 4851 | CA | VAL | 629 | 59.828 | 1.610 | 15.315 | 1.00 | 25.34 |
| ATOM | 4852 | CB | VAL | 629 | 58.812 | 0.693 | 16.007 | 1.00 | 21.26 |
| ATOM | 4853 | CG1 | VAL | 629 | 59.492 | -0.604 | 16.412 | 1.00 | 22.96 |
| ATOM | 4854 | CG2 | VAL | 629 | 58.205 | 1.398 | 17.207 | 1.00 | 16.65 |
| ATOM | 4855 | C | VAL | 629 | 60.266 | 0.962 | 14.007 | 1.00 | 26.79 |
| ATOM | 4856 | O | VAL | 629 | 59.454 | 0.839 | 13.087 | 1.00 | 28.60 |
| ATOM | 4857 | N | LEU | 630 | 61.542 | 0.603 | 13.904 | 1.00 | 25.91 |
| ATOM | 4859 | CA | LEU | 630 | 62.062 | -0.021 | 12.685 | 1.00 | 26.95 |
| ATOM | 4860 | CB | LEU | 630 | 63.297 | 0.733 | 12.210 | 1.00 | 22.79 |
| ATOM | 4861 | CG | LEU | 630 | 63.044 | 2.242 | 12.111 | 1.00 | 20.04 |
| ATOM | 4862 | CD1 | LEU | 630 | 64.345 | 2.944 | 11.972 | 1.00 | 11.86 |
| ATOM | 4863 | CD2 | LEU | 630 | 62.111 | 2.603 | 10.965 | 1.00 | 19.22 |
| ATOM | 4864 | C | LEU | 630 | 62.367 | -1.492 | 12.961 | 1.00 | 28.01 |
| ATOM | 4865 | O | LEU | 630 | 62.629 | -1.852 | 14.101 | 1.00 | 28.26 |
| ATOM | 4866 | N | VAL | 631 | 62.246 | -2.346 | 11.946 | 1.00 | 30.82 |
| ATOM | 4868 | CA | VAL | 631 | 62.468 | -3.790 | 12.098 | 1.00 | 31.75 |
| ATOM | 4869 | CB | VAL | 631 | 61.194 | -4.607 | 11.659 | 1.00 | 30.04 |
| ATOM | 4870 | CG1 | VAL | 631 | 61.346 | -6.085 | 12.026 | 1.00 | 29.25 |
| ATOM | 4871 | CG2 | VAL | 631 | 59.937 | -4.030 | 12.290 | 1.00 | 24.59 |
| ATOM | 4872 | C | VAL | 631 | 63.697 | -4.286 | 11.305 | 1.00 | 35.24 |
| ATOM | 4873 | O | VAL | 631 | 63.849 | -3.999 | 10.097 | 1.00 | 34.02 |
| ATOM | 4874 | N | THR | 632 | 64.551 | -5.052 | 11.979 | 1.00 | 36.24 |
| ATOM | 4876 | CA | THR | 632 | 65.770 | -5.574 | 11.365 | 1.00 | 38.23 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4877 | CB | THR | 632 | 66.843 | -5.836 | 12.416 | 1.00 | 38.21 |
| ATOM | 4878 | OG1 | THR | 632 | 66.423 | -6.908 | 13.272 | 1.00 | 38.31 |
| ATOM | 4880 | CG2 | THR | 632 | 67.069 | -4.582 | 13.238 | 1.00 | 40.22 |
| ATOM | 4881 | C | THR | 632 | 65.526 | -6.854 | 10.593 | 1.00 | 39.17 |
| ATOM | 4882 | O | THR | 632 | 64.471 | -7.457 | 10.744 | 1.00 | 41.26 |
| ATOM | 4883 | N | GLU | 633 | 66.496 | -7.259 | 9.766 | 1.00 | 41.23 |
| ATOM | 4885 | CA | GLU | 633 | 66.397 | -8.483 | 8.960 | 1.00 | 42.62 |
| ATOM | 4886 | CB | GLU | 633 | 67.677 | -8.712 | 8.154 | 1.00 | 44.25 |
| ATOM | 4887 | CG | GLU | 633 | 67.610 | -9.884 | 7.154 | 1.00 | 51.05 |
| ATOM | 4888 | CD | GLU | 633 | 66.825 | -9.594 | 5.858 | 1.00 | 56.28 |
| ATOM | 4889 | OE1 | GLU | 633 | 66.390 | -8.444 | 5.626 | 1.00 | 62.64 |
| ATOM | 4890 | OE2 | GLU | 633 | 66.651 | -10.536 | 5.058 | 1.00 | 58.41 |
| ATOM | 4891 | C | GLU | 633 | 66.097 | -9.722 | 9.797 | 1.00 | 41.83 |
| ATOM | 4892 | O | GLU | 633 | 65.578 | -10.704 | 9.288 | 1.00 | 42.77 |
| ATOM | 4893 | N | ASP | 634 | 66.415 | -9.665 | 11.082 | 1.00 | 43.14 |
| ATOM | 4895 | CA | ASP | 634 | 66.167 | -10.784 | 11.978 | 1.00 | 44.01 |
| ATOM | 4896 | CB | ASP | 634 | 67.361 | -11.007 | 12.914 | 1.00 | 49.37 |
| ATOM | 4897 | CG | ASP | 634 | 68.636 | -11.396 | 12.166 | 1.00 | 54.70 |
| ATOM | 4898 | OD1 | ASP | 634 | 68.683 | -12.515 | 11.595 | 1.00 | 55.43 |
| ATOM | 4899 | OD2 | ASP | 634 | 69.602 | -10.596 | 12.167 | 1.00 | 56.17 |
| ATOM | 4900 | C | ASP | 634 | 64.925 | -10.507 | 12.801 | 1.00 | 43.95 |
| ATOM | 4901 | O | ASP | 634 | 64.754 | -11.085 | 13.864 | 1.00 | 45.92 |
| ATOM | 4902 | N | ASN | 635 | 64.075 | -9.604 | 12.316 | 1.00 | 44.71 |
| ATOM | 4904 | CA | ASN | 635 | 62.822 | -9.220 | 12.980 | 1.00 | 43.07 |
| ATOM | 4905 | CB | ASN | 635 | 61.854 | -10.404 | 13.018 | 1.00 | 45.50 |
| ATOM | 4906 | CG | ASN | 635 | 61.606 | -10.994 | 11.653 | 1.00 | 45.43 |
| ATOM | 4907 | OD1 | ASN | 635 | 60.997 | -10.369 | 10.788 | 1.00 | 49.56 |
| ATOM | 4908 | ND2 | ASN | 635 | 62.114 | -12.190 | 11.435 | 1.00 | 48.18 |
| ATOM | 4911 | C | ASN | 635 | 62.927 | -8.609 | 14.380 | 1.00 | 41.64 |
| ATOM | 4912 | O | ASN | 635 | 62.050 | -8.814 | 15.221 | 1.00 | 41.69 |
| ATOM | 4913 | N | VAL | 636 | 63.984 | -7.843 | 14.627 | 1.00 | 41.17 |
| ATOM | 4915 | CA | VAL | 636 | 64.177 | -7.178 | 15.922 | 1.00 | 39.01 |
| ATOM | 4916 | CB | VAL | 636 | 65.692 | -7.002 | 16.259 | 1.00 | 40.66 |
| ATOM | 4917 | CG1 | VAL | 636 | 65.882 | -6.209 | 17.560 | 1.00 | 35.04 |
| ATOM | 4918 | CG2 | VAL | 636 | 66.355 | -8.360 | 16.367 | 1.00 | 41.69 |
| ATOM | 4919 | C | VAL | 636 | 63.544 | -5.789 | 15.925 | 1.00 | 36.77 |
| ATOM | 4920 | O | VAL | 636 | 63.817 | -4.989 | 15.045 | 1.00 | 38.35 |
| ATOM | 4921 | N | MET | 637 | 62.696 | -5.518 | 16.908 | 1.00 | 35.71 |
| ATOM | 4923 | CA | MET | 637 | 62.049 | -4.216 | 17.031 | 1.00 | 33.65 |
| ATOM | 4924 | CB | MET | 637 | 60.783 | -4.319 | 17.884 | 1.00 | 38.24 |
| ATOM | 4925 | CG | MET | 637 | 59.737 | -5.314 | 17.371 | 1.00 | 41.34 |
| ATOM | 4926 | SD | MET | 637 | 59.128 | -4.993 | 15.695 | 1.00 | 42.24 |
| ATOM | 4927 | CE | MET | 637 | 59.249 | -6.621 | 14.976 | 1.00 | 39.27 |
| ATOM | 4928 | C | MET | 637 | 63.001 | -3.209 | 17.668 | 1.00 | 32.62 |
| ATOM | 4929 | O | MET | 637 | 63.524 | -3.436 | 18.765 | 1.00 | 30.56 |
| ATOM | 4930 | N | LYS | 638 | 63.173 | -2.070 | 17.008 | 1.00 | 32.03 |
| ATOM | 4932 | CA | LYS | 638 | 64.073 | -1.027 | 17.492 | 1.00 | 28.77 |
| ATOM | 4933 | CB | LYS | 638 | 65.351 | -1.022 | 16.654 | 1.00 | 27.71 |
| ATOM | 4934 | CG | LYS | 638 | 66.245 | -2.211 | 16.896 | 1.00 | 25.04 |
| ATOM | 4935 | CD | LYS | 638 | 67.429 | -2.170 | 15.976 | 1.00 | 24.50 |
| ATOM | 4936 | CE | LYS | 638 | 68.443 | -3.187 | 16.390 | 1.00 | 22.85 |
| ATOM | 4937 | NZ | LYS | 638 | 69.121 | -2.803 | 17.651 | 1.00 | 24.79 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4941 | C | LYS | 638 | 63.443 | 0.364 | 17.446 | 1.00 | 28.00 |
| ATOM | 4942 | O | LYS | 638 | 62.977 | 0.799 | 16.391 | 1.00 | 25.60 |
| ATOM | 4943 | N | ILE | 639 | 63.410 | 1.032 | 18.601 | 1.00 | 25.32 |
| ATOM | 4945 | CA | ILE | 639 | 62.857 | 2.379 | 18.721 | 1.00 | 25.91 |
| ATOM | 4946 | CB | ILE | 639 | 62.800 | 2.875 | 20.201 | 1.00 | 25.56 |
| ATOM | 4947 | CG2 | ILE | 639 | 62.074 | 4.208 | 20.279 | 1.00 | 22.82 |
| ATOM | 4948 | CG1 | ILE | 639 | 62.142 | 1.835 | 21.118 | 1.00 | 28.00 |
| ATOM | 4949 | CD1 | ILE | 639 | 60.634 | 1.748 | 21.003 | 1.00 | 33.25 |
| ATOM | 4950 | C | ILE | 639 | 63.739 | 3.363 | 17.955 | 1.00 | 26.87 |
| ATOM | 4951 | O | ILE | 639 | 64.968 | 3.381 | 18.125 | 1.00 | 24.13 |
| ATOM | 4952 | N | ALA | 640 | 63.108 | 4.170 | 17.108 | 1.00 | 26.74 |
| ATOM | 4954 | CA | ALA | 640 | 63.825 | 5.176 | 16.339 | 1.00 | 30.62 |
| ATOM | 4955 | CB | ALA | 640 | 63.624 | 4.939 | 14.851 | 1.00 | 30.31 |
| ATOM | 4956 | C | ALA | 640 | 63.338 | 6.572 | 16.739 | 1.00 | 32.53 |
| ATOM | 4957 | O | ALA | 640 | 62.289 | 6.706 | 17.371 | 1.00 | 33.83 |
| ATOM | 4958 | N | ASP | 641 | 64.082 | 7.605 | 16.351 | 1.00 | 33.05 |
| ATOM | 4960 | CA | ASP | 641 | 63.749 | 9.010 | 16.656 | 1.00 | 37.66 |
| ATOM | 4961 | CB | ASP | 641 | 62.539 | 9.489 | 15.840 | 1.00 | 42.62 |
| ATOM | 4962 | CG | ASP | 641 | 62.928 | 10.026 | 14.471 | 1.00 | 50.92 |
| ATOM | 4963 | OD1 | ASP | 641 | 64.092 | 9.833 | 14.021 | 1.00 | 59.21 |
| ATOM | 4964 | OD2 | ASP | 641 | 62.063 | 10.652 | 13.823 | 1.00 | 54.05 |
| ATOM | 4965 | C | ASP | 641 | 63.545 | 9.367 | 18.125 | 1.00 | 37.85 |
| ATOM | 4966 | O | ASP | 641 | 62.805 | 10.294 | 18.448 | 1.00 | 39.10 |
| ATOM | 4967 | N | PHE | 642 | 64.204 | 8.635 | 19.016 | 1.00 | 37.47 |
| ATOM | 4969 | CA | PHE | 642 | 64.099 | 8.874 | 20.456 | 1.00 | 36.47 |
| ATOM | 4970 | CB | PHE | 642 | 64.403 | 7.581 | 21.226 | 1.00 | 32.22 |
| ATOM | 4971 | CG | PHE | 642 | 65.786 | 7.013 | 20.964 | 1.00 | 30.65 |
| ATOM | 4972 | CD1 | PHE | 642 | 66.906 | 7.537 | 21.607 | 1.00 | 32.45 |
| ATOM | 4973 | CD2 | PHE | 642 | 65.969 | 5.981 | 20.054 | 1.00 | 28.53 |
| ATOM | 4974 | CE1 | PHE | 642 | 68.180 | 7.050 | 21.342 | 1.00 | 30.88 |
| ATOM | 4975 | CE2 | PHE | 642 | 67.234 | 5.494 | 19.789 | 1.00 | 27.74 |
| ATOM | 4976 | CZ | PHE | 642 | 68.344 | 6.027 | 20.431 | 1.00 | 29.64 |
| ATOM | 4977 | C | PHE | 642 | 65.050 | 10.001 | 20.907 | 1.00 | 39.69 |
| ATOM | 4978 | O | PHE | 642 | 64.967 | 10.469 | 22.047 | 1.00 | 38.22 |
| ATOM | 4979 | N | GLY | 643 | 65.966 | 10.400 | 20.015 | 1.00 | 41.08 |
| ATOM | 4981 | CA | GLY | 643 | 66.925 | 11.447 | 20.324 | 1.00 | 40.65 |
| ATOM | 4982 | C | GLY | 643 | 66.694 | 12.747 | 19.571 | 1.00 | 43.53 |
| ATOM | 4983 | O | GLY | 643 | 67.500 | 13.666 | 19.688 | 1.00 | 41.10 |
| ATOM | 4984 | N | LEU | 644 | 65.617 | 12.825 | 18.786 | 1.00 | 48.35 |
| ATOM | 4986 | CA | LEU | 644 | 65.306 | 14.034 | 18.019 | 1.00 | 51.11 |
| ATOM | 4987 | CB | LEU | 644 | 63.962 | 13.907 | 17.314 | 1.00 | 50.28 |
| ATOM | 4988 | CG | LEU | 644 | 63.900 | 13.059 | 16.057 | 1.00 | 54.03 |
| ATOM | 4989 | CD1 | LEU | 644 | 62.541 | 13.278 | 15.413 | 1.00 | 57.34 |
| ATOM | 4990 | CD2 | LEU | 644 | 65.006 | 13.467 | 15.105 | 1.00 | 56.95 |
| ATOM | 4991 | C | LEU | 644 | 65.248 | 15.257 | 18.894 | 1.00 | 52.68 |
| ATOM | 4992 | O | LEU | 644 | 64.850 | 15.175 | 20.053 | 1.00 | 54.95 |
| ATOM | 4993 | N | ALA | 645 | 65.629 | 16.399 | 18.332 | 1.00 | 54.61 |
| ATOM | 4995 | CA | ALA | 645 | 65.610 | 17.656 | 19.073 | 1.00 | 54.60 |
| ATOM | 4996 | CB | ALA | 645 | 66.495 | 18.684 | 18.382 | 1.00 | 53.32 |
| ATOM | 4997 | C | ALA | 645 | 64.178 | 18.185 | 19.215 | 1.00 | 54.09 |
| ATOM | 4998 | O | ALA | 645 | 63.716 | 18.488 | 20.322 | 1.00 | 53.14 |
| ATOM | 4999 | N | ASP | 652 | 52.340 | 21.795 | 14.895 | 1.00 | 91.33 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5001 | CA | ASP | 652 | 51.194 | 21.914 | 14.004 | 1.00 | 90.97 |
| ATOM | 5002 | CB | ASP | 652 | 51.650 | 22.138 | 12.555 | 1.00 | 92.06 |
| ATOM | 5003 | CG | ASP | 652 | 50.488 | 22.434 | 11.606 | 1.00 | 94.00 |
| ATOM | 5004 | OD1 | ASP | 652 | 49.479 | 23.032 | 12.042 | 1.00 | 95.25 |
| ATOM | 5005 | OD2 | ASP | 652 | 50.586 | 22.075 | 10.414 | 1.00 | 94.81 |
| ATOM | 5006 | C | ASP | 652 | 50.352 | 20.652 | 14.103 | 1.00 | 90.61 |
| ATOM | 5007 | O | ASP | 652 | 50.645 | 19.641 | 13.463 | 1.00 | 91.26 |
| ATOM | 5008 | N | TYR | 653 | 49.289 | 20.737 | 14.895 | 1.00 | 89.65 |
| ATOM | 5010 | CA | TYR | 653 | 48.381 | 19.619 | 15.110 | 1.00 | 88.25 |
| ATOM | 5011 | CB | TYR | 653 | 47.306 | 20.003 | 16.133 | 1.00 | 88.16 |
| ATOM | 5012 | CG | TYR | 653 | 47.800 | 20.140 | 17.559 | 1.00 | 88.74 |
| ATOM | 5013 | CD1 | TYR | 653 | 47.047 | 20.818 | 18.513 | 1.00 | 90.00 |
| ATOM | 5014 | CE1 | TYR | 653 | 47.477 | 20.915 | 19.839 | 1.00 | 90.70 |
| ATOM | 5015 | CD2 | TYR | 653 | 49.006 | 19.559 | 17.964 | 1.00 | 89.14 |
| ATOM | 5016 | CE2 | TYR | 653 | 49.443 | 19.649 | 19.280 | 1.00 | 89.49 |
| ATOM | 5017 | CZ | TYR | 653 | 48.675 | 20.325 | 20.214 | 1.00 | 89.80 |
| ATOM | 5018 | OH | TYR | 653 | 49.109 | 20.394 | 21.518 | 1.00 | 89.81 |
| ATOM | 5020 | C | TYR | 653 | 47.701 | 19.165 | 13.830 | 1.00 | 87.32 |
| ATOM | 5021 | O | TYR | 653 | 47.180 | 18.057 | 13.759 | 1.00 | 87.70 |
| ATOM | 5022 | N | TYR | 654 | 47.734 | 20.013 | 12.814 | 1.00 | 86.51 |
| ATOM | 5024 | CA | TYR | 654 | 47.087 | 19.707 | 11.553 | 1.00 | 87.08 |
| ATOM | 5025 | CB | TYR | 654 | 46.387 | 20.959 | 11.028 | 1.00 | 88.45 |
| ATOM | 5026 | CG | TYR | 654 | 45.375 | 21.497 | 12.014 | 1.00 | 90.25 |
| ATOM | 5027 | CD1 | TYR | 654 | 45.781 | 22.017 | 13.246 | 1.00 | 90.15 |
| ATOM | 5028 | CE1 | TYR | 654 | 44.857 | 22.431 | 14.197 | 1.00 | 90.94 |
| ATOM | 5029 | CD2 | TYR | 654 | 44.012 | 21.419 | 11.753 | 1.00 | 91.22 |
| ATOM | 5030 | CE2 | TYR | 654 | 43.078 | 21.833 | 12.698 | 1.00 | 93.22 |
| ATOM | 5031 | CZ | TYR | 654 | 43.506 | 22.335 | 13.918 | 1.00 | 92.39 |
| ATOM | 5032 | OH | TYR | 654 | 42.588 | 22.717 | 14.872 | 1.00 | 94.38 |
| ATOM | 5034 | C | TYR | 654 | 48.012 | 19.115 | 10.503 | 1.00 | 87.34 |
| ATOM | 5035 | O | TYR | 654 | 47.567 | 18.767 | 9.410 | 1.00 | 88.29 |
| ATOM | 5036 | N | LYS | 655 | 49.290 | 18.971 | 10.836 | 1.00 | 86.67 |
| ATOM | 5038 | CA | LYS | 655 | 50.233 | 18.406 | 9.887 | 1.00 | 87.62 |
| ATOM | 5039 | CB | LYS | 655 | 51.666 | 18.814 | 10.229 | 1.00 | 90.01 |
| ATOM | 5040 | CG | LYS | 655 | 52.688 | 18.252 | 9.251 | 1.00 | 95.23 |
| ATOM | 5041 | CD | LYS | 655 | 54.106 | 18.646 | 9.607 | 1.00 | 99.04 |
| ATOM | 5042 | CE | LYS | 655 | 55.108 | 17.832 | 8.789 | 1.00 | 102.26 |
| ATOM | 5043 | NZ | LYS | 655 | 56.528 | 18.184 | 9.099 | 1.00 | 104.44 |
| ATOM | 5047 | C | LYS | 655 | 50.102 | 16.890 | 9.896 | 1.00 | 87.61 |
| ATOM | 5048 | O | LYS | 655 | 50.233 | 16.259 | 10.945 | 1.00 | 87.58 |
| ATOM | 5049 | N | LYS | 656 | 49.787 | 16.319 | 8.737 | 1.00 | 87.88 |
| ATOM | 5051 | CA | LYS | 656 | 49.639 | 14.875 | 8.603 | 1.00 | 89.03 |
| ATOM | 5052 | CB | LYS | 656 | 48.795 | 14.537 | 7.376 | 1.00 | 90.44 |
| ATOM | 5053 | CG | LYS | 656 | 47.313 | 14.802 | 7.535 | 1.00 | 93.30 |
| ATOM | 5054 | CD | LYS | 656 | 46.590 | 14.599 | 6.213 | 1.00 | 96.87 |
| ATOM | 5055 | CE | LYS | 656 | 45.089 | 14.555 | 6.406 | 1.00 | 99.35 |
| ATOM | 5056 | NZ | LYS | 656 | 44.362 | 14.518 | 5.106 | 1.00 | 102.42 |
| ATOM | 5060 | C | LYS | 656 | 51.004 | 14.206 | 8.487 | 1.00 | 88.57 |
| ATOM | 5061 | O | LYS | 656 | 51.915 | 14.749 | 7.855 | 1.00 | 88.38 |
| ATOM | 5062 | N | GLY | 660 | 49.270 | 10.021 | 5.735 | 1.00 | 61.58 |
| ATOM | 5064 | CA | GLY | 660 | 48.416 | 11.168 | 6.005 | 1.00 | 58.75 |
| ATOM | 5065 | C | GLY | 660 | 47.664 | 11.092 | 7.324 | 1.00 | 57.22 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5066 | O | GLY | 660 | 46.555 | 11.624 | 7.437 | 1.00 | 58.01 |
| ATOM | 5067 | N | ARG | 661 | 48.231 | 10.374 | 8.293 | 1.00 | 55.37 |
| ATOM | 5069 | CA | ARG | 661 | 47.631 | 10.247 | 9.622 | 1.00 | 51.19 |
| ATOM | 5070 | CB | ARG | 661 | 48.095 | 8.965 | 10.337 | 1.00 | 51.89 |
| ATOM | 5071 | CG | ARG | 661 | 47.756 | 7.663 | 9.612 | 1.00 | 51.56 |
| ATOM | 5072 | CD | ARG | 661 | 48.057 | 6.443 | 10.484 | 1.00 | 50.77 |
| ATOM | 5073 | NE | ARG | 661 | 47.834 | 5.181 | 9.772 | 1.00 | 50.04 |
| ATOM | 5075 | CZ | ARG | 661 | 48.015 | 3.974 | 10.307 | 1.00 | 48.12 |
| ATOM | 5076 | NH1 | ARG | 661 | 48.421 | 3.855 | 11.569 | 1.00 | 43.28 |
| ATOM | 5079 | NH2 | ARG | 661 | 47.788 | 2.882 | 9.578 | 1.00 | 43.69 |
| ATOM | 5082 | C | ARG | 661 | 48.041 | 11.463 | 10.446 | 1.00 | 46.22 |
| ATOM | 5083 | O | ARG | 661 | 48.998 | 12.162 | 10.097 | 1.00 | 44.78 |
| ATOM | 5084 | N | LEU | 662 | 47.328 | 11.703 | 11.542 | 1.00 | 41.80 |
| ATOM | 5086 | CA | LEU | 662 | 47.621 | 12.837 | 12.419 | 1.00 | 36.78 |
| ATOM | 5087 | CB | LEU | 662 | 46.342 | 13.596 | 12.758 | 1.00 | 33.05 |
| ATOM | 5088 | CG | LEU | 662 | 45.642 | 14.279 | 11.585 | 1.00 | 28.24 |
| ATOM | 5089 | CD1 | LEU | 662 | 44.198 | 14.611 | 11.935 | 1.00 | 24.66 |
| ATOM | 5090 | CD2 | LEU | 662 | 46.429 | 15.511 | 11.217 | 1.00 | 28.35 |
| ATOM | 5091 | C | LEU | 662 | 48.278 | 12.328 | 13.695 | 1.00 | 36.10 |
| ATOM | 5092 | O | LEU | 662 | 47.695 | 11.521 | 14.431 | 1.00 | 34.46 |
| ATOM | 5093 | N | PRO | 663 | 49.526 | 12.751 | 13.945 | 1.00 | 35.83 |
| ATOM | 5094 | CD | PRO | 663 | 50.360 | 13.537 | 13.022 | 1.00 | 37.72 |
| ATOM | 5095 | CA | PRO | 663 | 50.310 | 12.365 | 15.119 | 1.00 | 35.68 |
| ATOM | 5096 | CB | PRO | 663 | 51.611 | 13.130 | 14.914 | 1.00 | 35.23 |
| ATOM | 5097 | CG | PRO | 663 | 51.756 | 13.134 | 13.437 | 1.00 | 36.10 |
| ATOM | 5098 | C | PRO | 663 | 49.660 | 12.703 | 16.453 | 1.00 | 35.87 |
| ATOM | 5099 | O | PRO | 663 | 49.958 | 12.069 | 17.469 | 1.00 | 39.86 |
| ATOM | 5100 | N | VAL | 664 | 48.787 | 13.705 | 16.466 | 1.00 | 33.54 |
| ATOM | 5102 | CA | VAL | 664 | 48.109 | 14.076 | 17.699 | 1.00 | 31.24 |
| ATOM | 5103 | CB | VAL | 664 | 47.196 | 15.321 | 17.520 | 1.00 | 30.45 |
| ATOM | 5104 | CG1 | VAL | 664 | 48.025 | 16.480 | 17.051 | 1.00 | 32.54 |
| ATOM | 5105 | CG2 | VAL | 664 | 46.093 | 15.062 | 16.523 | 1.00 | 34.77 |
| ATOM | 5106 | C | VAL | 664 | 47.301 | 12.895 | 18.233 | 1.00 | 31.33 |
| ATOM | 5107 | O | VAL | 664 | 47.095 | 12.782 | 19.438 | 1.00 | 32.66 |
| ATOM | 5108 | N | LYS | 665 | 46.940 | 11.968 | 17.345 | 1.00 | 30.44 |
| ATOM | 5110 | CA | LYS | 665 | 46.153 | 10.795 | 17.719 | 1.00 | 28.43 |
| ATOM | 5111 | CB | LYS | 665 | 45.596 | 10.133 | 16.466 | 1.00 | 24.82 |
| ATOM | 5112 | CG | LYS | 665 | 44.700 | 11.080 | 15.687 | 1.00 | 27.50 |
| ATOM | 5113 | CD | LYS | 665 | 44.096 | 10.466 | 14.442 | 1.00 | 26.62 |
| ATOM | 5114 | CE | LYS | 665 | 42.967 | 11.326 | 13.909 | 1.00 | 21.64 |
| ATOM | 5115 | NZ | LYS | 665 | 42.479 | 10.850 | 12.584 | 1.00 | 25.29 |
| ATOM | 5119 | C | LYS | 665 | 46.889 | 9.794 | 18.615 | 1.00 | 29.56 |
| ATOM | 5120 | O | LYS | 665 | 46.295 | 8.836 | 19.095 | 1.00 | 29.57 |
| ATOM | 5121 | N | TRP | 666 | 48.183 | 10.020 | 18.826 | 1.00 | 30.12 |
| ATOM | 5123 | CA | TRP | 666 | 48.987 | 9.174 | 19.704 | 1.00 | 31.39 |
| ATOM | 5124 | CB | TRP | 666 | 50.329 | 8.845 | 19.059 | 1.00 | 30.40 |
| ATOM | 5125 | CG | TRP | 666 | 50.263 | 7.700 | 18.106 | 1.00 | 30.79 |
| ATOM | 5126 | CD2 | TRP | 666 | 49.701 | 7.719 | 16.785 | 1.00 | 30.22 |
| ATOM | 5127 | CE2 | TRP | 666 | 49.891 | 6.430 | 16.245 | 1.00 | 28.24 |
| ATOM | 5128 | CE3 | TRP | 666 | 49.067 | 8.702 | 16.012 | 1.00 | 30.60 |
| ATOM | 5129 | CD1 | TRP | 666 | 50.743 | 6.435 | 18.307 | 1.00 | 28.07 |
| ATOM | 5130 | NE1 | TRP | 666 | 50.522 | 5.670 | 17.187 | 1.00 | 29.15 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5132 | CZ2 | TRP | 666 | 49.462 | 6.107 | 14.954 | 1.00 | 29.38 |
| ATOM | 5133 | CZ3 | TRP | 666 | 48.640 | 8.374 | 14.726 | 1.00 | 31.27 |
| ATOM | 5134 | CH2 | TRP | 666 | 48.845 | 7.086 | 14.213 | 1.00 | 31.33 |
| ATOM | 5135 | C | TRP | 666 | 49.242 | 9.902 | 21.026 | 1.00 | 33.92 |
| ATOM | 5136 | O | TRP | 666 | 49.591 | 9.287 | 22.040 | 1.00 | 35.23 |
| ATOM | 5137 | N | MET | 667 | 49.028 | 11.214 | 21.007 | 1.00 | 35.72 |
| ATOM | 5139 | CA | MET | 667 | 49.260 | 12.065 | 22.159 | 1.00 | 36.43 |
| ATOM | 5140 | CB | MET | 667 | 49.163 | 13.529 | 21.751 | 1.00 | 37.70 |
| ATOM | 5141 | CG | MET | 667 | 50.510 | 14.194 | 21.574 | 1.00 | 40.10 |
| ATOM | 5142 | SD | MET | 667 | 50.358 | 15.906 | 21.096 | 1.00 | 46.91 |
| ATOM | 5143 | CE | MET | 667 | 50.914 | 15.810 | 19.386 | 1.00 | 40.40 |
| ATOM | 5144 | C | MET | 667 | 48.389 | 11.839 | 23.378 | 1.00 | 38.36 |
| ATOM | 5145 | O | MET | 667 | 47.186 | 11.646 | 23.273 | 1.00 | 39.53 |
| ATOM | 5146 | N | ALA | 668 | 49.027 | 11.885 | 24.542 | 1.00 | 39.93 |
| ATOM | 5148 | CA | ALA | 668 | 48.345 | 11.733 | 25.815 | 1.00 | 38.48 |
| ATOM | 5149 | CB | ALA | 668 | 49.351 | 11.537 | 26.929 | 1.00 | 37.61 |
| ATOM | 5150 | C | ALA | 668 | 47.603 | 13.038 | 26.014 | 1.00 | 39.48 |
| ATOM | 5151 | O | ALA | 668 | 48.059 | 14.090 | 25.566 | 1.00 | 39.40 |
| ATOM | 5152 | N | PRO | 669 | 46.474 | 13.001 | 26.731 | 1.00 | 42.22 |
| ATOM | 5153 | CD | PRO | 669 | 45.842 | 11.827 | 27.355 | 1.00 | 42.77 |
| ATOM | 5154 | CA | PRO | 669 | 45.677 | 14.204 | 26.980 | 1.00 | 43.91 |
| ATOM | 5155 | CB | PRO | 669 | 44.609 | 13.698 | 27.948 | 1.00 | 44.49 |
| ATOM | 5156 | CG | PRO | 669 | 44.421 | 12.279 | 27.499 | 1.00 | 43.59 |
| ATOM | 5157 | C | PRO | 669 | 46.476 | 15.372 | 27.570 | 1.00 | 44.89 |
| ATOM | 5158 | O | PRO | 669 | 46.394 | 16.497 | 27.075 | 1.00 | 45.48 |
| ATOM | 5159 | N | GLU | 670 | 47.266 | 15.105 | 28.607 | 1.00 | 43.39 |
| ATOM | 5161 | CA | GLU | 670 | 48.050 | 16.158 | 29.244 | 1.00 | 42.97 |
| ATOM | 5162 | CB | GLU | 670 | 48.739 | 15.645 | 30.504 | 1.00 | 43.31 |
| ATOM | 5163 | CG | GLU | 670 | 49.864 | 14.646 | 30.252 | 1.00 | 44.78 |
| ATOM | 5164 | CD | GLU | 670 | 49.408 | 13.204 | 30.290 | 1.00 | 43.48 |
| ATOM | 5165 | OE1 | GLU | 670 | 50.225 | 12.331 | 30.639 | 1.00 | 41.85 |
| ATOM | 5166 | OE2 | GLU | 670 | 48.235 | 12.931 | 29.986 | 1.00 | 47.18 |
| ATOM | 5167 | C | GLU | 670 | 49.090 | 16.798 | 28.333 | 1.00 | 43.18 |
| ATOM | 5168 | O | GLU | 670 | 49.362 | 17.983 | 28.444 | 1.00 | 41.68 |
| ATOM | 5169 | N | ALA | 671 | 49.677 | 16.008 | 27.440 | 1.00 | 44.65 |
| ATOM | 5171 | CA | ALA | 671 | 50.686 | 16.512 | 26.513 | 1.00 | 44.44 |
| ATOM | 5172 | CB | ALA | 671 | 51.412 | 15.347 | 25.841 | 1.00 | 40.17 |
| ATOM | 5173 | C | ALA | 671 | 50.046 | 17.410 | 25.465 | 1.00 | 46.49 |
| ATOM | 5174 | O | ALA | 671 | 50.558 | 18.484 | 25.148 | 1.00 | 45.70 |
| ATOM | 5175 | N | LEU | 672 | 48.903 | 16.970 | 24.952 | 1.00 | 50.30 |
| ATOM | 5177 | CA | LEU | 672 | 48.163 | 17.702 | 23.925 | 1.00 | 52.07 |
| ATOM | 5178 | CB | LEU | 672 | 47.080 | 16.782 | 23.335 | 1.00 | 54.41 |
| ATOM | 5179 | CG | LEU | 672 | 46.388 | 17.103 | 22.005 | 1.00 | 57.12 |
| ATOM | 5180 | CD1 | LEU | 672 | 47.404 | 17.316 | 20.912 | 1.00 | 57.65 |
| ATOM | 5181 | CD2 | LEU | 672 | 45.459 | 15.951 | 21.640 | 1.00 | 56.14 |
| ATOM | 5182 | C | LEU | 672 | 47.535 | 18.964 | 24.512 | 1.00 | 52.42 |
| ATOM | 5183 | O | LEU | 672 | 47.683 | 20.058 | 23.969 | 1.00 | 52.71 |
| ATOM | 5184 | N | PHE | 673 | 46.863 | 18.803 | 25.645 | 1.00 | 52.74 |
| ATOM | 5186 | CA | PHE | 673 | 46.203 | 19.911 | 26.314 | 1.00 | 54.32 |
| ATOM | 5187 | CB | PHE | 673 | 44.995 | 19.394 | 27.104 | 1.00 | 52.92 |
| ATOM | 5188 | CG | PHE | 673 | 43.987 | 18.646 | 26.259 | 1.00 | 52.38 |
| ATOM | 5189 | CD1 | PHE | 673 | 43.399 | 17.477 | 26.728 | 1.00 | 53.49 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5190 | CD2 | PHE | 673 | 43.624 | 19.109 | 24.999 | 1.00 | 51.61 |
| ATOM | 5191 | CE1 | PHE | 673 | 42.468 | 16.779 | 25.957 | 1.00 | 50.49 |
| ATOM | 5192 | CE2 | PHE | 673 | 42.698 | 18.420 | 24.229 | 1.00 | 50.91 |
| ATOM | 5193 | CZ | PHE | 673 | 42.118 | 17.250 | 24.710 | 1.00 | 50.09 |
| ATOM | 5194 | C | PHE | 673 | 47.138 | 20.732 | 27.220 | 1.00 | 56.29 |
| ATOM | 5195 | O | PHE | 673 | 47.289 | 21.938 | 27.026 | 1.00 | 58.05 |
| ATOM | 5196 | N | ASP | 674 | 47.808 | 20.076 | 28.165 | 1.00 | 56.38 |
| ATOM | 5198 | CA | ASP | 674 | 48.703 | 20.772 | 29.104 | 1.00 | 56.12 |
| ATOM | 5199 | CB | ASP | 674 | 48.644 | 20.101 | 30.485 | 1.00 | 53.81 |
| ATOM | 5200 | CG | ASP | 674 | 47.299 | 20.234 | 31.152 | 1.00 | 52.48 |
| ATOM | 5201 | OD1 | ASP | 674 | 46.715 | 19.188 | 31.504 | 1.00 | 50.25 |
| ATOM | 5202 | OD2 | ASP | 674 | 46.844 | 21.384 | 31.337 | 1.00 | 51.16 |
| ATOM | 5203 | C | ASP | 674 | 50.182 | 20.886 | 28.706 | 1.00 | 57.07 |
| ATOM | 5204 | O | ASP | 674 | 51.010 | 21.273 | 29.541 | 1.00 | 56.00 |
| ATOM | 5205 | N | ARG | 675 | 50.525 | 20.526 | 27.468 | 1.00 | 57.28 |
| ATOM | 5207 | CA | ARG | 675 | 51.915 | 20.576 | 26.995 | 1.00 | 55.64 |
| ATOM | 5208 | CB | ARG | 675 | 52.341 | 22.020 | 26.692 | 1.00 | 58.95 |
| ATOM | 5209 | CG | ARG | 675 | 51.542 | 22.678 | 25.569 | 1.00 | 66.91 |
| ATOM | 5210 | CD | ARG | 675 | 52.082 | 24.066 | 25.202 | 1.00 | 72.90 |
| ATOM | 5211 | NE | ARG | 675 | 53.360 | 24.019 | 24.482 | 1.00 | 75.10 |
| ATOM | 5213 | CZ | ARG | 675 | 54.096 | 25.089 | 24.181 | 1.00 | 73.61 |
| ATOM | 5214 | NH1 | ARG | 675 | 53.687 | 26.301 | 24.536 | 1.00 | 71.27 |
| ATOM | 5217 | NH2 | ARG | 675 | 55.250 | 24.943 | 23.540 | 1.00 | 72.12 |
| ATOM | 5220 | C | ARG | 675 | 52.853 | 19.932 | 28.017 | 1.00 | 53.25 |
| ATOM | 5221 | O | ARG | 675 | 53.988 | 20.366 | 28.211 | 1.00 | 52.13 |
| ATOM | 5222 | N | ILE | 676 | 52.359 | 18.883 | 28.664 | 1.00 | 51.44 |
| ATOM | 5224 | CA | ILE | 676 | 53.108 | 18.153 | 29.683 | 1.00 | 49.81 |
| ATOM | 5225 | CB | ILE | 676 | 52.241 | 17.944 | 30.958 | 1.00 | 46.07 |
| ATOM | 5226 | CG2 | ILE | 676 | 52.804 | 16.844 | 31.856 | 1.00 | 40.98 |
| ATOM | 5227 | CG1 | ILE | 676 | 52.129 | 19.257 | 31.721 | 1.00 | 43.31 |
| ATOM | 5228 | CD1 | ILE | 676 | 51.324 | 19.147 | 32.963 | 1.00 | 45.02 |
| ATOM | 5229 | C | ILE | 676 | 53.572 | 16.800 | 29.144 | 1.00 | 51.20 |
| ATOM | 5230 | O | ILE | 676 | 52.770 | 15.892 | 28.951 | 1.00 | 52.37 |
| ATOM | 5231 | N | TYR | 677 | 54.865 | 16.675 | 28.890 | 1.00 | 52.81 |
| ATOM | 5233 | CA | TYR | 677 | 55.412 | 15.429 | 28.383 | 1.00 | 53.96 |
| ATOM | 5234 | CB | TYR | 677 | 56.296 | 15.700 | 27.167 | 1.00 | 57.26 |
| ATOM | 5235 | CG | TYR | 677 | 55.524 | 16.175 | 25.951 | 1.00 | 64.10 |
| ATOM | 5236 | CD1 | TYR | 677 | 55.229 | 17.532 | 25.762 | 1.00 | 65.60 |
| ATOM | 5237 | CE1 | TYR | 677 | 54.514 | 17.965 | 24.634 | 1.00 | 67.15 |
| ATOM | 5238 | CD2 | TYR | 677 | 55.085 | 15.263 | 24.985 | 1.00 | 66.29 |
| ATOM | 5239 | CE2 | TYR | 677 | 54.376 | 15.680 | 23.862 | 1.00 | 67.34 |
| ATOM | 5240 | CZ | TYR | 677 | 54.095 | 17.028 | 23.692 | 1.00 | 69.24 |
| ATOM | 5241 | OH | TYR | 677 | 53.399 | 17.414 | 22.573 | 1.00 | 73.55 |
| ATOM | 5243 | C | TYR | 677 | 56.192 | 14.713 | 29.482 | 1.00 | 52.30 |
| ATOM | 5244 | O | TYR | 677 | 57.053 | 15.309 | 30.124 | 1.00 | 53.73 |
| ATOM | 5245 | N | THR | 678 | 55.830 | 13.461 | 29.748 | 1.00 | 48.95 |
| ATOM | 5247 | CA | THR | 678 | 56.505 | 12.659 | 30.760 | 1.00 | 45.99 |
| ATOM | 5248 | CB | THR | 678 | 55.729 | 12.634 | 32.107 | 1.00 | 46.04 |
| ATOM | 5249 | OG1 | THR | 678 | 54.663 | 11.676 | 32.046 | 1.00 | 49.79 |
| ATOM | 5251 | CG2 | THR | 678 | 55.160 | 14.010 | 32.429 | 1.00 | 45.58 |
| ATOM | 5252 | C | THR | 678 | 56.656 | 11.221 | 30.261 | 1.00 | 43.81 |
| ATOM | 5253 | O | THR | 678 | 56.231 | 10.888 | 29.158 | 1.00 | 45.12 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5254 | N | HIS | 679 | 57.250 | 10.359 | 31.076 | 1.00 | 41.50 |
| ATOM | 5256 | CA | HIS | 679 | 57.414 | 8.971 | 30.687 | 1.00 | 38.39 |
| ATOM | 5257 | CB | HIS | 679 | 58.390 | 8.253 | 31.603 | 1.00 | 38.62 |
| ATOM | 5258 | CG | HIS | 679 | 59.798 | 8.770 | 31.524 | 1.00 | 41.51 |
| ATOM | 5259 | CD2 | HIS | 679 | 60.456 | 9.690 | 32.273 | 1.00 | 40.12 |
| ATOM | 5260 | ND1 | HIS | 679 | 60.715 | 8.296 | 30.613 | 1.00 | 41.18 |
| ATOM | 5262 | CE1 | HIS | 679 | 61.880 | 8.892 | 30.806 | 1.00 | 39.44 |
| ATOM | 5263 | NE2 | HIS | 679 | 61.747 | 9.742 | 31.807 | 1.00 | 41.37 |
| ATOM | 5265 | C | HIS | 679 | 56.068 | 8.279 | 30.720 | 1.00 | 39.57 |
| ATOM | 5266 | O | HIS | 679 | 55.909 | 7.215 | 30.137 | 1.00 | 41.93 |
| ATOM | 5267 | N | GLN | 680 | 55.108 | 8.863 | 31.429 | 1.00 | 39.84 |
| ATOM | 5269 | CA | GLN | 680 | 53.773 | 8.290 | 31.483 | 1.00 | 38.92 |
| ATOM | 5270 | CB | GLN | 680 | 53.021 | 8.705 | 32.751 | 1.00 | 38.21 |
| ATOM | 5271 | CG | GLN | 680 | 53.518 | 8.005 | 34.022 | 1.00 | 42.17 |
| ATOM | 5272 | CD | GLN | 680 | 53.651 | 6.477 | 33.878 | 1.00 | 43.35 |
| ATOM | 5273 | OE1 | GLN | 680 | 52.686 | 5.737 | 34.056 | 1.00 | 44.05 |
| ATOM | 5274 | NE2 | GLN | 680 | 54.860 | 6.010 | 33.564 | 1.00 | 37.17 |
| ATOM | 5277 | C | GLN | 680 | 53.012 | 8.674 | 30.221 | 1.00 | 39.33 |
| ATOM | 5278 | O | GLN | 680 | 52.220 | 7.883 | 29.709 | 1.00 | 40.26 |
| ATOM | 5279 | N | SER | 681 | 53.299 | 9.854 | 29.673 | 1.00 | 38.00 |
| ATOM | 5281 | CA | SER | 681 | 52.636 | 10.251 | 28.441 | 1.00 | 37.44 |
| ATOM | 5282 | CB | SER | 681 | 52.963 | 11.698 | 28.078 | 1.00 | 37.67 |
| ATOM | 5283 | OG | SER | 681 | 54.349 | 11.937 | 28.102 | 1.00 | 38.03 |
| ATOM | 5285 | C | SER | 681 | 53.095 | 9.278 | 27.356 | 1.00 | 38.28 |
| ATOM | 5286 | O | SER | 681 | 52.302 | 8.866 | 26.510 | 1.00 | 39.41 |
| ATOM | 5287 | N | ASP | 682 | 54.362 | 8.866 | 27.431 | 1.00 | 36.81 |
| ATOM | 5289 | CA | ASP | 682 | 54.920 | 7.888 | 26.495 | 1.00 | 36.41 |
| ATOM | 5290 | CB | ASP | 682 | 56.404 | 7.655 | 26.765 | 1.00 | 37.18 |
| ATOM | 5291 | CG | ASP | 682 | 57.309 | 8.584 | 25.968 | 1.00 | 40.08 |
| ATOM | 5292 | OD1 | ASP | 682 | 58.528 | 8.317 | 25.959 | 1.00 | 41.94 |
| ATOM | 5293 | OD2 | ASP | 682 | 56.824 | 9.565 | 25.352 | 1.00 | 39.55 |
| ATOM | 5294 | C | ASP | 682 | 54.180 | 6.561 | 26.645 | 1.00 | 36.93 |
| ATOM | 5295 | O | ASP | 682 | 54.005 | 5.818 | 25.675 | 1.00 | 38.23 |
| ATOM | 5296 | N | VAL | 683 | 53.742 | 6.268 | 27.866 | 1.00 | 36.33 |
| ATOM | 5298 | CA | VAL | 683 | 53.000 | 5.040 | 28.143 | 1.00 | 36.29 |
| ATOM | 5299 | CB | VAL | 683 | 52.834 | 4.820 | 29.683 | 1.00 | 35.29 |
| ATOM | 5300 | CG1 | VAL | 683 | 51.900 | 3.653 | 29.989 | 1.00 | 34.98 |
| ATOM | 5301 | CG2 | VAL | 683 | 54.198 | 4.546 | 30.312 | 1.00 | 30.55 |
| ATOM | 5302 | C | VAL | 683 | 51.648 | 5.067 | 27.392 | 1.00 | 35.21 |
| ATOM | 5303 | O | VAL | 683 | 51.223 | 4.050 | 26.845 | 1.00 | 32.81 |
| ATOM | 5304 | N | TRP | 684 | 51.027 | 6.245 | 27.309 | 1.00 | 34.49 |
| ATOM | 5306 | CA | TRP | 684 | 49.759 | 6.412 | 26.602 | 1.00 | 36.39 |
| ATOM | 5307 | CB | TRP | 684 | 49.200 | 7.825 | 26.811 | 1.00 | 39.30 |
| ATOM | 5308 | CG | TRP | 684 | 48.006 | 8.174 | 25.947 | 1.00 | 41.47 |
| ATOM | 5309 | CD2 | TRP | 684 | 46.651 | 8.381 | 26.384 | 1.00 | 42.41 |
| ATOM | 5310 | CE2 | TRP | 684 | 45.896 | 8.744 | 25.247 | 1.00 | 41.76 |
| ATOM | 5311 | CE3 | TRP | 684 | 46.004 | 8.298 | 27.627 | 1.00 | 42.06 |
| ATOM | 5312 | CD1 | TRP | 684 | 48.010 | 8.410 | 24.597 | 1.00 | 40.55 |
| ATOM | 5313 | NE1 | TRP | 684 | 46.749 | 8.756 | 24.175 | 1.00 | 42.32 |
| ATOM | 5315 | CZ2 | TRP | 684 | 44.522 | 9.022 | 25.315 | 1.00 | 41.35 |
| ATOM | 5316 | CZ3 | TRP | 684 | 44.638 | 8.576 | 27.692 | 1.00 | 41.99 |
| ATOM | 5317 | CH2 | TRP | 684 | 43.917 | 8.933 | 26.541 | 1.00 | 41.07 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5318 | C | TRP | 684 | 49.964 | 6.125 | 25.115 | 1.00 | 36.12 |
| ATOM | 5319 | O | TRP | 684 | 49.152 | 5.410 | 24.511 | 1.00 | 38.69 |
| ATOM | 5320 | N | SER | 685 | 51.029 | 6.690 | 24.534 | 1.00 | 33.48 |
| ATOM | 5322 | CA | SER | 685 | 51.395 | 6.491 | 23.130 | 1.00 | 26.49 |
| ATOM | 5323 | CB | SER | 685 | 52.636 | 7.300 | 22.802 | 1.00 | 23.40 |
| ATOM | 5324 | OG | SER | 685 | 52.403 | 8.688 | 22.992 | 1.00 | 30.31 |
| ATOM | 5326 | C | SER | 685 | 51.665 | 5.015 | 22.859 | 1.00 | 26.25 |
| ATOM | 5327 | O | SER | 685 | 51.377 | 4.510 | 21.782 | 1.00 | 28.78 |
| ATOM | 5328 | N | PHE | 686 | 52.214 | 4.319 | 23.846 | 1.00 | 28.14 |
| ATOM | 5330 | CA | PHE | 686 | 52.470 | 2.884 | 23.727 | 1.00 | 28.53 |
| ATOM | 5331 | CB | PHE | 686 | 53.245 | 2.399 | 24.947 | 1.00 | 27.34 |
| ATOM | 5332 | CG | PHE | 686 | 53.567 | 0.937 | 24.917 | 1.00 | 29.91 |
| ATOM | 5333 | CD1 | PHE | 686 | 54.424 | 0.419 | 23.942 | 1.00 | 29.23 |
| ATOM | 5334 | CD2 | PHE | 686 | 53.016 | 0.075 | 25.861 | 1.00 | 28.28 |
| ATOM | 5335 | CE1 | PHE | 686 | 54.725 | -0.936 | 23.908 | 1.00 | 27.65 |
| ATOM | 5336 | CE2 | PHE | 686 | 53.307 | -1.274 | 25.840 | 1.00 | 27.18 |
| ATOM | 5337 | CZ | PHE | 686 | 54.166 | -1.787 | 24.861 | 1.00 | 30.06 |
| ATOM | 5338 | C | PHE | 686 | 51.129 | 2.117 | 23.618 | 1.00 | 31.42 |
| ATOM | 5339 | O | PHE | 686 | 51.041 | 1.096 | 22.930 | 1.00 | 29.05 |
| ATOM | 5340 | N | GLY | 687 | 50.093 | 2.623 | 24.298 | 1.00 | 31.18 |
| ATOM | 5342 | CA | GLY | 687 | 48.783 | 2.000 | 24.258 | 1.00 | 32.16 |
| ATOM | 5343 | C | GLY | 687 | 48.276 | 2.026 | 22.825 | 1.00 | 35.09 |
| ATOM | 5344 | O | GLY | 687 | 47.805 | 1.011 | 22.289 | 1.00 | 36.38 |
| ATOM | 5345 | N | VAL | 688 | 48.378 | 3.188 | 22.186 | 1.00 | 33.72 |
| ATOM | 5347 | CA | VAL | 688 | 47.949 | 3.307 | 20.808 | 1.00 | 30.28 |
| ATOM | 5348 | CB | VAL | 688 | 47.996 | 4.761 | 20.322 | 1.00 | 28.62 |
| ATOM | 5349 | CG1 | VAL | 688 | 47.433 | 4.862 | 18.905 | 1.00 | 26.79 |
| ATOM | 5350 | CG2 | VAL | 688 | 47.202 | 5.645 | 21.275 | 1.00 | 26.40 |
| ATOM | 5351 | C | VAL | 688 | 48.823 | 2.406 | 19.930 | 1.00 | 30.01 |
| ATOM | 5352 | O | VAL | 688 | 48.324 | 1.782 | 18.989 | 1.00 | 30.37 |
| ATOM | 5353 | N | LEU | 689 | 50.108 | 2.282 | 20.273 | 1.00 | 29.76 |
| ATOM | 5355 | CA | LEU | 689 | 51.022 | 1.418 | 19.510 | 1.00 | 29.37 |
| ATOM | 5356 | CB | LEU | 689 | 52.476 | 1.577 | 19.982 | 1.00 | 25.78 |
| ATOM | 5357 | CG | LEU | 689 | 53.564 | 0.944 | 19.097 | 1.00 | 23.00 |
| ATOM | 5358 | CD1 | LEU | 689 | 54.855 | 1.741 | 19.153 | 1.00 | 24.44 |
| ATOM | 5359 | CD2 | LEU | 689 | 53.823 | -0.471 | 19.479 | 1.00 | 21.63 |
| ATOM | 5360 | C | LEU | 689 | 50.583 | -0.043 | 19.634 | 1.00 | 29.98 |
| ATOM | 5361 | O | LEU | 689 | 50.708 | -0.806 | 18.678 | 1.00 | 28.75 |
| ATOM | 5362 | N | LEU | 690 | 50.048 | -0.409 | 20.803 | 1.00 | 32.38 |
| ATOM | 5364 | CA | LEU | 690 | 49.562 | -1.764 | 21.060 | 1.00 | 32.66 |
| ATOM | 5365 | CB | LEU | 690 | 49.114 | -1.929 | 22.517 | 1.00 | 32.33 |
| ATOM | 5366 | CG | LEU | 690 | 50.107 | -2.192 | 23.658 | 1.00 | 32.00 |
| ATOM | 5367 | CD1 | LEU | 690 | 49.330 | -2.201 | 24.962 | 1.00 | 35.74 |
| ATOM | 5368 | CD2 | LEU | 690 | 50.834 | -3.513 | 23.475 | 1.00 | 30.76 |
| ATOM | 5369 | C | LEU | 690 | 48.369 | -2.018 | 20.156 | 1.00 | 33.29 |
| ATOM | 5370 | O | LEU | 690 | 48.248 | -3.079 | 19.550 | 1.00 | 35.08 |
| ATOM | 5371 | N | TRP | 691 | 47.490 | -1.026 | 20.065 | 1.00 | 34.28 |
| ATOM | 5373 | CA | TRP | 691 | 46.304 | -1.114 | 19.221 | 1.00 | 33.79 |
| ATOM | 5374 | CB | TRP | 691 | 45.483 | 0.172 | 19.364 | 1.00 | 32.68 |
| ATOM | 5375 | CG | TRP | 691 | 44.147 | 0.144 | 18.669 | 1.00 | 31.23 |
| ATOM | 5376 | CD2 | TRP | 691 | 43.888 | 0.490 | 17.312 | 1.00 | 28.11 |
| ATOM | 5377 | CE2 | TRP | 691 | 42.506 | 0.310 | 17.089 | 1.00 | 29.96 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5378 | CE3 | TRP | 691 | 44.686 | 0.949 | 16.257 | 1.00 | 28.70 |
| ATOM | 5379 | CD1 | TRP | 691 | 42.936 | -0.225 | 19.208 | 1.00 | 29.37 |
| ATOM | 5380 | NE1 | TRP | 691 | 41.951 | -0.130 | 18.265 | 1.00 | 30.89 |
| ATOM | 5382 | CZ2 | TRP | 691 | 41.909 | 0.555 | 15.845 | 1.00 | 29.50 |
| ATOM | 5383 | CZ3 | TRP | 691 | 44.093 | 1.194 | 15.021 | 1.00 | 27.43 |
| ATOM | 5384 | CH2 | TRP | 691 | 42.719 | 1.002 | 14.830 | 1.00 | 29.27 |
| ATOM | 5385 | C | TRP | 691 | 46.744 | -1.319 | 17.763 | 1.00 | 34.12 |
| ATOM | 5386 | O | TRP | 691 | 46.139 | -2.088 | 17.029 | 1.00 | 33.88 |
| ATOM | 5387 | N | GLU | 692 | 47.817 | -0.636 | 17.366 | 1.00 | 36.37 |
| ATOM | 5389 | CA | GLU | 692 | 48.355 | -0.723 | 16.010 | 1.00 | 35.35 |
| ATOM | 5390 | CB | GLU | 692 | 49.532 | 0.233 | 15.826 | 1.00 | 31.75 |
| ATOM | 5391 | CG | GLU | 692 | 49.138 | 1.694 | 15.746 | 1.00 | 32.63 |
| ATOM | 5392 | CD | GLU | 692 | 50.318 | 2.585 | 15.403 | 1.00 | 35.28 |
| ATOM | 5393 | OE1 | GLU | 692 | 51.150 | 2.847 | 16.301 | 1.00 | 37.81 |
| ATOM | 5394 | OE2 | GLU | 692 | 50.430 | 3.017 | 14.237 | 1.00 | 34.85 |
| ATOM | 5395 | C | GLU | 692 | 48.810 | -2.118 | 15.658 | 1.00 | 35.71 |
| ATOM | 5396 | O | GLU | 692 | 48.589 | -2.570 | 14.544 | 1.00 | 37.26 |
| ATOM | 5397 | N | ILE | 693 | 49.439 | -2.798 | 16.610 | 1.00 | 35.05 |
| ATOM | 5399 | CA | ILE | 693 | 49.944 | -4.153 | 16.396 | 1.00 | 35.00 |
| ATOM | 5400 | CB | ILE | 693 | 50.843 | -4.608 | 17.575 | 1.00 | 35.88 |
| ATOM | 5401 | CG2 | ILE | 693 | 51.275 | -6.064 | 17.400 | 1.00 | 36.03 |
| ATOM | 5402 | CG1 | ILE | 693 | 52.081 | -3.711 | 17.669 | 1.00 | 34.66 |
| ATOM | 5403 | CD1 | ILE | 693 | 52.814 | -3.874 | 18.943 | 1.00 | 35.52 |
| ATOM | 5404 | C | ILE | 693 | 48.810 | -5.153 | 16.232 | 1.00 | 34.29 |
| ATOM | 5405 | O | ILE | 693 | 48.790 | -5.943 | 15.281 | 1.00 | 33.66 |
| ATOM | 5406 | N | PHE | 694 | 47.837 | -5.079 | 17.127 | 1.00 | 34.44 |
| ATOM | 5408 | CA | PHE | 694 | 46.722 | -5.999 | 17.082 | 1.00 | 35.63 |
| ATOM | 5409 | CB | PHE | 694 | 46.156 | -6.167 | 18.490 | 1.00 | 35.26 |
| ATOM | 5410 | CG | PHE | 694 | 47.158 | -6.787 | 19.428 | 1.00 | 35.26 |
| ATOM | 5411 | CD1 | PHE | 694 | 47.796 | -6.017 | 20.389 | 1.00 | 33.07 |
| ATOM | 5412 | CD2 | PHE | 694 | 47.574 | -8.111 | 19.237 | 1.00 | 31.74 |
| ATOM | 5413 | CE1 | PHE | 694 | 48.837 | -6.539 | 21.137 | 1.00 | 31.01 |
| ATOM | 5414 | CE2 | PHE | 694 | 48.614 | -8.643 | 19.982 | 1.00 | 31.64 |
| ATOM | 5415 | CZ | PHE | 694 | 49.254 | -7.855 | 20.934 | 1.00 | 31.84 |
| ATOM | 5416 | C | PHE | 694 | 45.688 | -5.771 | 15.986 | 1.00 | 36.62 |
| ATOM | 5417 | O | PHE | 694 | 44.844 | -6.632 | 15.729 | 1.00 | 38.73 |
| ATOM | 5418 | N | THR | 695 | 45.781 | -4.626 | 15.313 | 1.00 | 35.76 |
| ATOM | 5420 | CA | THR | 695 | 44.898 | -4.331 | 14.191 | 1.00 | 34.86 |
| ATOM | 5421 | CB | THR | 695 | 44.245 | -2.929 | 14.298 | 1.00 | 32.81 |
| ATOM | 5422 | OG1 | THR | 695 | 45.246 | -1.909 | 14.211 | 1.00 | 31.61 |
| ATOM | 5424 | CG2 | THR | 695 | 43.497 | -2.795 | 15.603 | 1.00 | 29.90 |
| ATOM | 5425 | C | THR | 695 | 45.766 | -4.426 | 12.934 | 1.00 | 35.95 |
| ATOM | 5426 | O | THR | 695 | 45.333 | -4.064 | 11.841 | 1.00 | 38.88 |
| ATOM | 5427 | N | LEU | 696 | 46.993 | -4.919 | 13.119 | 1.00 | 34.68 |
| ATOM | 5429 | CA | LEU | 696 | 47.979 | -5.100 | 12.053 | 1.00 | 32.84 |
| ATOM | 5430 | CB | LEU | 696 | 47.622 | -6.294 | 11.161 | 1.00 | 32.65 |
| ATOM | 5431 | CG | LEU | 696 | 47.493 | -7.657 | 11.838 | 1.00 | 30.89 |
| ATOM | 5432 | CD1 | LEU | 696 | 47.315 | -8.734 | 10.785 | 1.00 | 31.30 |
| ATOM | 5433 | CD2 | LEU | 696 | 48.718 | -7.939 | 12.659 | 1.00 | 30.76 |
| ATOM | 5434 | C | LEU | 696 | 48.280 | -3.872 | 11.197 | 1.00 | 32.43 |
| ATOM | 5435 | O | LEU | 696 | 48.259 | -3.931 | 9.965 | 1.00 | 31.48 |
| ATOM | 5436 | N | GLY | 697 | 48.597 | -2.768 | 11.867 | 1.00 | 33.65 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5438 | CA | GLY | 697 | 48.940 | -1.529 | 11.188 | 1.00 | 32.78 |
| ATOM | 5439 | C | GLY | 697 | 47.742 | -0.641 | 10.960 | 1.00 | 33.06 |
| ATOM | 5440 | O | GLY | 697 | 47.728 | 0.172 | 10.048 | 1.00 | 34.74 |
| ATOM | 5441 | N | GLY | 698 | 46.719 | -0.798 | 11.782 | 1.00 | 35.53 |
| ATOM | 5443 | CA | GLY | 698 | 45.531 | 0.009 | 11.612 | 1.00 | 36.87 |
| ATOM | 5444 | C | GLY | 698 | 45.771 | 1.496 | 11.753 | 1.00 | 34.92 |
| ATOM | 5445 | O | GLY | 698 | 46.779 | 1.926 | 12.299 | 1.00 | 34.08 |
| ATOM | 5446 | N | SER | 699 | 44.814 | 2.271 | 11.265 | 1.00 | 36.45 |
| ATOM | 5448 | CA | SER | 699 | 44.858 | 3.725 | 11.318 | 1.00 | 35.36 |
| ATOM | 5449 | CB | SER | 699 | 44.363 | 4.290 | 9.995 | 1.00 | 34.58 |
| ATOM | 5450 | OG | SER | 699 | 44.126 | 5.684 | 10.087 | 1.00 | 41.43 |
| ATOM | 5452 | C | SER | 699 | 43.927 | 4.146 | 12.451 | 1.00 | 36.53 |
| ATOM | 5453 | O | SER | 699 | 42.734 | 3.812 | 12.438 | 1.00 | 37.58 |
| ATOM | 5454 | N | PRO | 700 | 44.471 | 4.799 | 13.491 | 1.00 | 36.03 |
| ATOM | 5455 | CD | PRO | 700 | 45.896 | 5.028 | 13.776 | 1.00 | 34.58 |
| ATOM | 5456 | CA | PRO | 700 | 43.630 | 5.228 | 14.611 | 1.00 | 35.47 |
| ATOM | 5457 | CB | PRO | 700 | 44.655 | 5.573 | 15.694 | 1.00 | 34.59 |
| ATOM | 5458 | CG | PRO | 700 | 45.840 | 5.990 | 14.919 | 1.00 | 34.18 |
| ATOM | 5459 | C | PRO | 700 | 42.742 | 6.411 | 14.247 | 1.00 | 34.66 |
| ATOM | 5460 | O | PRO | 700 | 43.194 | 7.363 | 13.616 | 1.00 | 34.39 |
| ATOM | 5461 | N | TYR | 701 | 41.462 | 6.293 | 14.588 | 1.00 | 34.11 |
| ATOM | 5463 | CA | TYR | 701 | 40.459 | 7.324 | 14.338 | 1.00 | 33.11 |
| ATOM | 5464 | CB | TYR | 701 | 40.713 | 8.548 | 15.225 | 1.00 | 38.13 |
| ATOM | 5465 | CG | TYR | 701 | 40.552 | 8.272 | 16.706 | 1.00 | 43.52 |
| ATOM | 5466 | CD1 | TYR | 701 | 41.538 | 8.637 | 17.616 | 1.00 | 44.79 |
| ATOM | 5467 | CE1 | TYR | 701 | 41.387 | 8.391 | 18.978 | 1.00 | 49.99 |
| ATOM | 5468 | CD2 | TYR | 701 | 39.405 | 7.647 | 17.197 | 1.00 | 47.59 |
| ATOM | 5469 | CE2 | TYR | 701 | 39.245 | 7.395 | 18.552 | 1.00 | 49.15 |
| ATOM | 5470 | CZ | TYR | 701 | 40.237 | 7.770 | 19.444 | 1.00 | 50.84 |
| ATOM | 5471 | OH | TYR | 701 | 40.091 | 7.539 | 20.804 | 1.00 | 54.00 |
| ATOM | 5473 | C | TYR | 701 | 40.389 | 7.736 | 12.877 | 1.00 | 30.95 |
| ATOM | 5474 | O | TYR | 701 | 40.597 | 8.900 | 12.534 | 1.00 | 30.64 |
| ATOM | 5475 | N | PRO | 702 | 40.096 | 6.773 | 11.985 | 1.00 | 30.06 |
| ATOM | 5476 | CD | PRO | 702 | 39.887 | 5.336 | 12.192 | 1.00 | 25.47 |
| ATOM | 5477 | CA | PRO | 702 | 40.014 | 7.112 | 10.561 | 1.00 | 29.36 |
| ATOM | 5478 | CB | PRO | 702 | 39.836 | 5.744 | 9.899 | 1.00 | 25.86 |
| ATOM | 5479 | CG | PRO | 702 | 39.185 | 4.946 | 10.929 | 1.00 | 24.42 |
| ATOM | 5480 | C | PRO | 702 | 38.859 | 8.045 | 10.256 | 1.00 | 31.49 |
| ATOM | 5481 | O | PRO | 702 | 37.716 | 7.794 | 10.654 | 1.00 | 33.50 |
| ATOM | 5482 | N | GLY | 703 | 39.194 | 9.151 | 9.592 | 1.00 | 30.85 |
| ATOM | 5484 | CA | GLY | 703 | 38.210 | 10.149 | 9.212 | 1.00 | 27.67 |
| ATOM | 5485 | C | GLY | 703 | 37.985 | 11.230 | 10.250 | 1.00 | 27.39 |
| ATOM | 5486 | O | GLY | 703 | 37.270 | 12.194 | 9.981 | 1.00 | 26.56 |
| ATOM | 5487 | N | VAL | 704 | 38.627 | 11.100 | 11.412 | 1.00 | 27.05 |
| ATOM | 5489 | CA | VAL | 704 | 38.466 | 12.053 | 12.505 | 1.00 | 28.50 |
| ATOM | 5490 | CB | VAL | 704 | 38.576 | 11.364 | 13.876 | 1.00 | 28.95 |
| ATOM | 5491 | CG1 | VAL | 704 | 38.509 | 12.397 | 14.990 | 1.00 | 29.36 |
| ATOM | 5492 | CG2 | VAL | 704 | 37.475 | 10.338 | 14.045 | 1.00 | 29.64 |
| ATOM | 5493 | C | VAL | 704 | 39.473 | 13.194 | 12.493 | 1.00 | 30.95 |
| ATOM | 5494 | O | VAL | 704 | 40.669 | 12.977 | 12.661 | 1.00 | 32.90 |
| ATOM | 5495 | N | PRO | 705 | 39.001 | 14.428 | 12.269 | 1.00 | 31.09 |
| ATOM | 5496 | CD | PRO | 705 | 37.682 | 14.795 | 11.728 | 1.00 | 31.49 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5497 | CA | PRO | 705 | 39.926 | 15.561 | 12.255 | 1.00 | 29.66 |
| ATOM | 5498 | CB | PRO | 705 | 39.152 | 16.618 | 11.477 | 1.00 | 30.16 |
| ATOM | 5499 | CG | PRO | 705 | 37.720 | 16.289 | 11.778 | 1.00 | 33.76 |
| ATOM | 5500 | C | PRO | 705 | 40.334 | 16.028 | 13.654 | 1.00 | 29.25 |
| ATOM | 5501 | O | PRO | 705 | 39.693 | 15.695 | 14.659 | 1.00 | 24.77 |
| ATOM | 5502 | N | VAL | 706 | 41.396 | 16.828 | 13.690 | 1.00 | 32.40 |
| ATOM | 5504 | CA | VAL | 706 | 41.976 | 17.355 | 14.929 | 1.00 | 36.51 |
| ATOM | 5505 | CB | VAL | 706 | 43.023 | 18.450 | 14.629 | 1.00 | 36.79 |
| ATOM | 5506 | CG1 | VAL | 706 | 43.680 | 18.903 | 15.914 | 1.00 | 37.79 |
| ATOM | 5507 | CG2 | VAL | 706 | 44.058 | 17.942 | 13.653 | 1.00 | 37.26 |
| ATOM | 5508 | C | VAL | 706 | 40.977 | 17.915 | 15.943 | 1.00 | 38.21 |
| ATOM | 5509 | O | VAL | 706 | 41.052 | 17.600 | 17.130 | 1.00 | 37.65 |
| ATOM | 5510 | N | GLU | 707 | 40.060 | 18.754 | 15.467 | 1.00 | 40.27 |
| ATOM | 5512 | CA | GLU | 707 | 39.045 | 19.360 | 16.324 | 1.00 | 40.57 |
| ATOM | 5513 | CB | GLU | 707 | 38.186 | 20.324 | 15.499 | 1.00 | 40.56 |
| ATOM | 5514 | C | GLU | 707 | 38.164 | 18.288 | 16.958 | 1.00 | 41.60 |
| ATOM | 5515 | O | GLU | 707 | 37.871 | 18.323 | 18.158 | 1.00 | 41.79 |
| ATOM | 5516 | N | GLU | 708 | 37.784 | 17.311 | 16.143 | 1.00 | 42.54 |
| ATOM | 5518 | CA | GLU | 708 | 36.947 | 16.210 | 16.576 | 1.00 | 44.09 |
| ATOM | 5519 | CB | GLU | 708 | 36.509 | 15.398 | 15.367 | 1.00 | 47.61 |
| ATOM | 5520 | CG | GLU | 708 | 35.687 | 16.219 | 14.381 | 1.00 | 50.42 |
| ATOM | 5521 | CD | GLU | 708 | 34.511 | 16.891 | 15.042 | 1.00 | 55.51 |
| ATOM | 5522 | OE1 | GLU | 708 | 33.856 | 16.249 | 15.899 | 1.00 | 58.91 |
| ATOM | 5523 | OE2 | GLU | 708 | 34.244 | 18.067 | 14.714 | 1.00 | 60.06 |
| ATOM | 5524 | C | GLU | 708 | 37.661 | 15.338 | 17.598 | 1.00 | 44.63 |
| ATOM | 5525 | O | GLU | 708 | 37.058 | 14.893 | 18.585 | 1.00 | 45.12 |
| ATOM | 5526 | N | LEU | 709 | 38.960 | 15.141 | 17.390 | 1.00 | 43.72 |
| ATOM | 5528 | CA | LEU | 709 | 39.768 | 14.346 | 18.312 | 1.00 | 39.85 |
| ATOM | 5529 | CB | LEU | 709 | 41.212 | 14.243 | 17.823 | 1.00 | 34.99 |
| ATOM | 5530 | CG | LEU | 709 | 42.037 | 13.359 | 18.756 | 1.00 | 31.80 |
| ATOM | 5531 | CD1 | LEU | 709 | 41.619 | 11.918 | 18.598 | 1.00 | 29.20 |
| ATOM | 5532 | CD2 | LEU | 709 | 43.495 | 13.533 | 18.454 | 1.00 | 31.19 |
| ATOM | 5533 | C | LEU | 709 | 39.751 | 15.001 | 19.683 | 1.00 | 39.26 |
| ATOM | 5534 | O | LEU | 709 | 39.646 | 14.317 | 20.714 | 1.00 | 37.71 |
| ATOM | 5535 | N | PHE | 710 | 39.872 | 16.327 | 19.691 | 1.00 | 38.62 |
| ATOM | 5537 | CA | PHE | 710 | 39.862 | 17.068 | 20.942 | 1.00 | 41.82 |
| ATOM | 5538 | CB | PHE | 710 | 40.016 | 18.567 | 20.688 | 1.00 | 42.02 |
| ATOM | 5539 | CG | PHE | 710 | 41.383 | 18.958 | 20.206 | 1.00 | 43.81 |
| ATOM | 5540 | CD1 | PHE | 710 | 42.441 | 18.043 | 20.242 | 1.00 | 47.07 |
| ATOM | 5541 | CD2 | PHE | 710 | 41.621 | 20.234 | 19.718 | 1.00 | 42.91 |
| ATOM | 5542 | CE1 | PHE | 710 | 43.716 | 18.401 | 19.793 | 1.00 | 49.22 |
| ATOM | 5543 | CE2 | PHE | 710 | 42.890 | 20.602 | 19.267 | 1.00 | 46.73 |
| ATOM | 5544 | CZ | PHE | 710 | 43.942 | 19.681 | 19.307 | 1.00 | 48.40 |
| ATOM | 5545 | C | PHE | 710 | 38.568 | 16.787 | 21.698 | 1.00 | 43.80 |
| ATOM | 5546 | O | PHE | 710 | 38.593 | 16.502 | 22.904 | 1.00 | 44.54 |
| ATOM | 5547 | N | LYS | 711 | 37.452 | 16.790 | 20.968 | 1.00 | 44.15 |
| ATOM | 5549 | CA | LYS | 711 | 36.148 | 16.539 | 21.569 | 1.00 | 42.60 |
| ATOM | 5550 | CB | LYS | 711 | 35.029 | 16.855 | 20.577 | 1.00 | 44.35 |
| ATOM | 5551 | CG | LYS | 711 | 33.661 | 16.781 | 21.200 | 1.00 | 48.05 |
| ATOM | 5552 | CD | LYS | 711 | 32.560 | 17.205 | 20.263 | 1.00 | 49.23 |
| ATOM | 5553 | CE | LYS | 711 | 31.212 | 16.804 | 20.855 | 1.00 | 50.61 |
| ATOM | 5554 | NZ | LYS | 711 | 30.078 | 17.204 | 19.987 | 1.00 | 56.56 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5558 | C | LYS | 711 | 36.045 | 15.105 | 22.084 | 1.00 | 41.50 |
| ATOM | 5559 | O | LYS | 711 | 35.589 | 14.875 | 23.202 | 1.00 | 41.06 |
| ATOM | 5560 | N | LEU | 712 | 36.489 | 14.144 | 21.282 | 1.00 | 41.61 |
| ATOM | 5562 | CA | LEU | 712 | 36.463 | 12.737 | 21.687 | 1.00 | 43.22 |
| ATOM | 5563 | CB | LEU | 712 | 37.070 | 11.841 | 20.600 | 1.00 | 41.69 |
| ATOM | 5564 | CG | LEU | 712 | 36.246 | 11.404 | 19.397 | 1.00 | 38.07 |
| ATOM | 5565 | CD1 | LEU | 712 | 37.071 | 10.460 | 18.527 | 1.00 | 34.55 |
| ATOM | 5566 | CD2 | LEU | 712 | 34.990 | 10.714 | 19.891 | 1.00 | 37.28 |
| ATOM | 5567 | C | LEU | 712 | 37.253 | 12.536 | 22.982 | 1.00 | 43.94 |
| ATOM | 5568 | O | LEU | 712 | 36.804 | 11.832 | 23.900 | 1.00 | 41.71 |
| ATOM | 5569 | N | LEU | 713 | 38.444 | 13.129 | 23.029 | 1.00 | 45.26 |
| ATOM | 5571 | CA | LEU | 713 | 39.318 | 13.022 | 24.191 | 1.00 | 46.47 |
| ATOM | 5572 | CB | LEU | 713 | 40.647 | 13.728 | 23.925 | 1.00 | 46.32 |
| ATOM | 5573 | CG | LEU | 713 | 41.524 | 13.012 | 22.889 | 1.00 | 44.05 |
| ATOM | 5574 | CD1 | LEU | 713 | 42.853 | 13.737 | 22.734 | 1.00 | 39.96 |
| ATOM | 5575 | CD2 | LEU | 713 | 41.758 | 11.571 | 23.328 | 1.00 | 41.78 |
| ATOM | 5576 | C | LEU | 713 | 38.665 | 13.519 | 25.477 | 1.00 | 47.50 |
| ATOM | 5577 | O | LEU | 713 | 38.630 | 12.789 | 26.472 | 1.00 | 48.26 |
| ATOM | 5578 | N | LYS | 714 | 38.098 | 14.725 | 25.440 | 1.00 | 47.08 |
| ATOM | 5580 | CA | LYS | 714 | 37.419 | 15.302 | 26.600 | 1.00 | 45.59 |
| ATOM | 5581 | CB | LYS | 714 | 36.974 | 16.727 | 26.293 | 1.00 | 47.53 |
| ATOM | 5582 | CG | LYS | 714 | 38.126 | 17.661 | 26.064 | 1.00 | 51.33 |
| ATOM | 5583 | CD | LYS | 714 | 37.647 | 19.044 | 25.689 | 1.00 | 59.12 |
| ATOM | 5584 | CE | LYS | 714 | 38.836 | 19.917 | 25.273 | 1.00 | 64.39 |
| ATOM | 5585 | NZ | LYS | 714 | 39.843 | 20.072 | 26.370 | 1.00 | 66.31 |
| ATOM | 5589 | C | LYS | 714 | 36.217 | 14.476 | 27.056 | 1.00 | 44.19 |
| ATOM | 5590 | O | LYS | 714 | 35.895 | 14.447 | 28.244 | 1.00 | 43.04 |
| ATOM | 5591 | N | GLU | 715 | 35.565 | 13.805 | 26.112 | 1.00 | 43.89 |
| ATOM | 5593 | CA | GLU | 715 | 34.401 | 12.976 | 26.424 | 1.00 | 44.12 |
| ATOM | 5594 | CB | GLU | 715 | 33.512 | 12.785 | 25.190 | 1.00 | 47.40 |
| ATOM | 5595 | CG | GLU | 715 | 32.860 | 14.053 | 24.623 | 1.00 | 52.31 |
| ATOM | 5596 | CD | GLU | 715 | 31.953 | 13.763 | 23.427 | 1.00 | 56.22 |
| ATOM | 5597 | OE1 | GLU | 715 | 32.121 | 12.699 | 22.784 | 1.00 | 57.16 |
| ATOM | 5598 | OE2 | GLU | 715 | 31.059 | 14.588 | 23.138 | 1.00 | 57.32 |
| ATOM | 5599 | C | GLU | 715 | 34.809 | 11.605 | 26.956 | 1.00 | 42.47 |
| ATOM | 5600 | O | GLU | 715 | 33.964 | 10.718 | 27.094 | 1.00 | 41.03 |
| ATOM | 5601 | N | GLY | 716 | 36.101 | 11.419 | 27.201 | 1.00 | 41.06 |
| ATOM | 5603 | CA | GLY | 716 | 36.593 | 10.150 | 27.718 | 1.00 | 41.58 |
| ATOM | 5604 | C | GLY | 716 | 36.548 | 8.985 | 26.739 | 1.00 | 41.60 |
| ATOM | 5605 | O | GLY | 716 | 36.640 | 7.816 | 27.141 | 1.00 | 38.34 |
| ATOM | 5606 | N | HIS | 717 | 36.469 | 9.303 | 25.450 | 1.00 | 42.80 |
| ATOM | 5608 | CA | HIS | 717 | 36.398 | 8.278 | 24.420 | 1.00 | 45.03 |
| ATOM | 5609 | CB | HIS | 717 | 36.082 | 8.894 | 23.052 | 1.00 | 46.28 |
| ATOM | 5610 | CG | HIS | 717 | 35.987 | 7.887 | 21.940 | 1.00 | 48.73 |
| ATOM | 5611 | CD2 | HIS | 717 | 34.941 | 7.157 | 21.483 | 1.00 | 48.67 |
| ATOM | 5612 | ND1 | HIS | 717 | 37.071 | 7.521 | 21.169 | 1.00 | 49.33 |
| ATOM | 5614 | CE1 | HIS | 717 | 36.701 | 6.607 | 20.290 | 1.00 | 45.65 |
| ATOM | 5615 | NE2 | HIS | 717 | 35.410 | 6.370 | 20.460 | 1.00 | 45.87 |
| ATOM | 5617 | C | HIS | 717 | 37.662 | 7.448 | 24.324 | 1.00 | 46.84 |
| ATOM | 5618 | O | HIS | 717 | 38.767 | 7.980 | 24.319 | 1.00 | 48.06 |
| ATOM | 5619 | N | ARG | 718 | 37.478 | 6.138 | 24.217 | 1.00 | 48.75 |
| ATOM | 5621 | CA | ARG | 718 | 38.573 | 5.181 | 24.091 | 1.00 | 49.16 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5622 | CB | ARG | 718 | 38.694 | 4.345 | 25.370 | 1.00 | 46.96 |
| ATOM | 5623 | CG | ARG | 718 | 39.005 | 5.164 | 26.617 | 1.00 | 49.78 |
| ATOM | 5624 | CD | ARG | 718 | 40.344 | 5.891 | 26.474 | 1.00 | 52.81 |
| ATOM | 5625 | NE | ARG | 718 | 40.724 | 6.639 | 27.672 | 1.00 | 52.99 |
| ATOM | 5627 | CZ | ARG | 718 | 40.598 | 7.961 | 27.817 | 1.00 | 53.38 |
| ATOM | 5628 | NH1 | ARG | 718 | 40.094 | 8.705 | 26.836 | 1.00 | 52.33 |
| ATOM | 5631 | NH2 | ARG | 718 | 41.025 | 8.553 | 28.928 | 1.00 | 49.30 |
| ATOM | 5634 | C | ARG | 718 | 38.257 | 4.293 | 22.878 | 1.00 | 50.73 |
| ATOM | 5635 | O | ARG | 718 | 37.086 | 4.003 | 22.601 | 1.00 | 51.78 |
| ATOM | 5636 | N | MET | 719 | 39.286 | 3.899 | 22.136 | 1.00 | 50.83 |
| ATOM | 5638 | CA | MET | 719 | 39.086 | 3.072 | 20.948 | 1.00 | 50.56 |
| ATOM | 5639 | CB | MET | 719 | 40.355 | 3.013 | 20.094 | 1.00 | 48.85 |
| ATOM | 5640 | CG | MET | 719 | 40.748 | 4.325 | 19.438 | 1.00 | 45.25 |
| ATOM | 5641 | SD | MET | 719 | 42.152 | 4.119 | 18.335 | 1.00 | 43.24 |
| ATOM | 5642 | CE | MET | 719 | 43.471 | 4.066 | 19.465 | 1.00 | 36.42 |
| ATOM | 5643 | C | MET | 719 | 38.649 | 1.671 | 21.312 | 1.00 | 51.07 |
| ATOM | 5644 | O | MET | 719 | 39.087 | 1.132 | 22.325 | 1.00 | 48.42 |
| ATOM | 5645 | N | ASP | 720 | 37.797 | 1.096 | 20.462 | 1.00 | 53.92 |
| ATOM | 5647 | CA | ASP | 720 | 37.254 | -0.253 | 20.648 | 1.00 | 55.90 |
| ATOM | 5648 | CB | ASP | 720 | 36.221 | -0.597 | 19.553 | 1.00 | 57.16 |
| ATOM | 5649 | CG | ASP | 720 | 34.998 | 0.320 | 19.552 | 1.00 | 59.05 |
| ATOM | 5650 | OD1 | ASP | 720 | 34.951 | 1.316 | 20.312 | 1.00 | 63.29 |
| ATOM | 5651 | OD2 | ASP | 720 | 34.074 | 0.042 | 18.758 | 1.00 | 54.85 |
| ATOM | 5652 | C | ASP | 720 | 38.326 | -1.343 | 20.638 | 1.00 | 55.89 |
| ATOM | 5653 | O | ASP | 720 | 39.397 | -1.190 | 20.027 | 1.00 | 55.28 |
| ATOM | 5654 | N | LYS | 721 | 38.008 | -2.450 | 21.304 | 1.00 | 56.09 |
| ATOM | 5656 | CA | LYS | 721 | 38.892 | -3.605 | 21.370 | 1.00 | 56.46 |
| ATOM | 5657 | CB | LYS | 721 | 38.344 | -4.606 | 22.378 | 1.00 | 58.16 |
| ATOM | 5658 | CG | LYS | 721 | 39.005 | -5.977 | 22.316 | 1.00 | 62.49 |
| ATOM | 5659 | CD | LYS | 721 | 38.449 | -6.873 | 23.401 | 1.00 | 66.40 |
| ATOM | 5660 | CE | LYS | 721 | 38.474 | -8.329 | 22.995 | 1.00 | 68.27 |
| ATOM | 5661 | NZ | LYS | 721 | 38.107 | -9.194 | 24.156 | 1.00 | 75.61 |
| ATOM | 5665 | C | LYS | 721 | 38.930 | -4.241 | 19.985 | 1.00 | 56.00 |
| ATOM | 5666 | O | LYS | 721 | 37.884 | -4.532 | 19.403 | 1.00 | 59.26 |
| ATOM | 5667 | N | PRO | 722 | 40.133 | -4.439 | 19.423 | 1.00 | 54.10 |
| ATOM | 5668 | CD | PRO | 722 | 41.461 | -3.968 | 19.836 | 1.00 | 53.72 |
| ATOM | 5669 | CA | PRO | 722 | 40.208 | -5.046 | 18.094 | 1.00 | 51.82 |
| ATOM | 5670 | CB | PRO | 722 | 41.702 | -4.953 | 17.759 | 1.00 | 49.09 |
| ATOM | 5671 | CG | PRO | 722 | 42.143 | -3.768 | 18.501 | 1.00 | 49.06 |
| ATOM | 5672 | C | PRO | 722 | 39.765 | -6.498 | 18.123 | 1.00 | 50.10 |
| ATOM | 5673 | O | PRO | 722 | 39.678 | -7.120 | 19.188 | 1.00 | 48.82 |
| ATOM | 5674 | N | SER | 723 | 39.453 | -7.020 | 16.945 | 1.00 | 49.87 |
| ATOM | 5676 | CA | SER | 723 | 39.079 | -8.410 | 16.814 | 1.00 | 50.27 |
| ATOM | 5677 | CB | SER | 723 | 38.396 | -8.643 | 15.473 | 1.00 | 48.56 |
| ATOM | 5678 | OG | SER | 723 | 39.273 | -8.323 | 14.404 | 1.00 | 48.93 |
| ATOM | 5680 | C | SER | 723 | 40.414 | -9.144 | 16.872 | 1.00 | 51.33 |
| ATOM | 5681 | O | SER | 723 | 41.400 | -8.679 | 16.311 | 1.00 | 51.18 |
| ATOM | 5682 | N | ASN | 724 | 40.445 | -10.284 | 17.551 | 1.00 | 54.65 |
| ATOM | 5684 | CA | ASN | 724 | 41.673 | -11.062 | 17.706 | 1.00 | 56.76 |
| ATOM | 5685 | CB | ASN | 724 | 42.370 | -11.286 | 16.359 | 1.00 | 58.96 |
| ATOM | 5686 | CG | ASN | 724 | 41.698 | -12.345 | 15.543 | 1.00 | 62.08 |
| ATOM | 5687 | OD1 | ASN | 724 | 41.645 | -13.508 | 15.948 | 1.00 | 67.56 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5688 | ND2 | ASN | 724 | 41.154 | -11.960 | 14.403 | 1.00 | 60.12 |
| ATOM | 5691 | C | ASN | 724 | 42.622 | -10.381 | 18.683 | 1.00 | 57.26 |
| ATOM | 5692 | O | ASN | 724 | 43.786 | -10.131 | 18.383 | 1.00 | 58.40 |
| ATOM | 5693 | N | CYS | 725 | 42.089 | -10.045 | 19.845 | 1.00 | 57.58 |
| ATOM | 5695 | CA | CYS | 725 | 42.852 | -9.418 | 20.908 | 1.00 | 57.02 |
| ATOM | 5696 | CB | CYS | 725 | 42.835 | -7.885 | 20.803 | 1.00 | 55.65 |
| ATOM | 5697 | SG | CYS | 725 | 43.782 | -7.034 | 22.119 | 1.00 | 52.17 |
| ATOM | 5698 | C | CYS | 725 | 42.158 | -9.884 | 22.177 | 1.00 | 56.53 |
| ATOM | 5699 | O | CYS | 725 | 40.927 | -9.954 | 22.240 | 1.00 | 55.99 |
| ATOM | 5700 | N | THR | 726 | 42.957 | -10.279 | 23.155 | 1.00 | 56.09 |
| ATOM | 5702 | CA | THR | 726 | 42.453 | -10.773 | 24.423 | 1.00 | 57.09 |
| ATOM | 5703 | CB | THR | 726 | 43.551 | -11.579 | 25.129 | 1.00 | 57.12 |
| ATOM | 5704 | OG1 | THR | 726 | 44.588 | -10.696 | 25.562 | 1.00 | 59.14 |
| ATOM | 5706 | CG2 | THR | 726 | 44.152 | -12.587 | 24.154 | 1.00 | 55.09 |
| ATOM | 5707 | C | THR | 726 | 41.994 | -9.608 | 25.288 | 1.00 | 57.58 |
| ATOM | 5708 | O | THR | 726 | 42.555 | -8.518 | 25.195 | 1.00 | 58.49 |
| ATOM | 5709 | N | ASN | 727 | 40.979 | -9.832 | 26.120 | 1.00 | 58.48 |
| ATOM | 5711 | CA | ASN | 727 | 40.482 | -8.774 | 26.986 | 1.00 | 58.74 |
| ATOM | 5712 | CB | ASN | 727 | 39.331 | -9.267 | 27.864 | 1.00 | 66.81 |
| ATOM | 5713 | CG | ASN | 727 | 39.674 | -10.534 | 28.631 | 1.00 | 76.72 |
| ATOM | 5714 | OD1 | ASN | 727 | 40.778 | -10.689 | 29.161 | 1.00 | 80.48 |
| ATOM | 5715 | ND2 | ASN | 727 | 38.716 | -11.458 | 28.689 | 1.00 | 82.39 |
| ATOM | 5718 | C | ASN | 727 | 41.606 | -8.238 | 27.852 | 1.00 | 55.48 |
| ATOM | 5719 | O | ASN | 727 | 41.589 | -7.080 | 28.255 | 1.00 | 51.24 |
| ATOM | 5720 | N | GLU | 728 | 42.589 | -9.099 | 28.114 | 1.00 | 55.37 |
| ATOM | 5722 | CA | GLU | 728 | 43.757 | -8.739 | 28.913 | 1.00 | 55.53 |
| ATOM | 5723 | CB | GLU | 728 | 44.611 | -9.983 | 29.198 | 1.00 | 55.75 |
| ATOM | 5724 | CG | GLU | 728 | 45.881 | -9.699 | 30.006 | 1.00 | 58.24 |
| ATOM | 5725 | CD | GLU | 728 | 46.606 | -10.958 | 30.463 | 1.00 | 58.16 |
| ATOM | 5726 | OE1 | GLU | 728 | 46.977 | -11.796 | 29.611 | 1.00 | 56.39 |
| ATOM | 5727 | OE2 | GLU | 728 | 46.816 | -11.102 | 31.686 | 1.00 | 58.35 |
| ATOM | 5728 | C | GLU | 728 | 44.564 | -7.685 | 28.153 | 1.00 | 54.11 |
| ATOM | 5729 | O | GLU | 728 | 44.790 | -6.575 | 28.654 | 1.00 | 55.67 |
| ATOM | 5730 | N | LEU | 729 | 44.954 | -8.020 | 26.926 | 1.00 | 49.65 |
| ATOM | 5732 | CA | LEU | 729 | 45.715 | -7.106 | 26.086 | 1.00 | 46.10 |
| ATOM | 5733 | CB | LEU | 729 | 46.038 | -7.766 | 24.742 | 1.00 | 39.77 |
| ATOM | 5734 | CG | LEU | 729 | 47.136 | -8.836 | 24.848 | 1.00 | 36.12 |
| ATOM | 5735 | CD1 | LEU | 729 | 47.118 | -9.757 | 23.673 | 1.00 | 34.89 |
| ATOM | 5736 | CD2 | LEU | 729 | 48.498 | -8.193 | 24.987 | 1.00 | 33.47 |
| ATOM | 5737 | C | LEU | 729 | 44.950 | -5.794 | 25.908 | 1.00 | 45.05 |
| ATOM | 5738 | O | LEU | 729 | 45.522 | -4.713 | 26.019 | 1.00 | 45.58 |
| ATOM | 5739 | N | TYR | 730 | 43.640 | -5.884 | 25.722 | 1.00 | 43.53 |
| ATOM | 5741 | CA | TYR | 730 | 42.831 | -4.692 | 25.557 | 1.00 | 43.57 |
| ATOM | 5742 | CB | TYR | 730 | 41.414 | -5.064 | 25.097 | 1.00 | 41.49 |
| ATOM | 5743 | CG | TYR | 730 | 40.492 | -3.870 | 24.951 | 1.00 | 40.28 |
| ATOM | 5744 | CD1 | TYR | 730 | 40.763 | -2.865 | 24.013 | 1.00 | 36.86 |
| ATOM | 5745 | CE1 | TYR | 730 | 39.937 | -1.752 | 23.891 | 1.00 | 36.21 |
| ATOM | 5746 | CD2 | TYR | 730 | 39.361 | -3.730 | 25.768 | 1.00 | 39.44 |
| ATOM | 5747 | CE2 | TYR | 730 | 38.522 | -2.616 | 25.654 | 1.00 | 38.13 |
| ATOM | 5748 | CZ | TYR | 730 | 38.817 | -1.632 | 24.712 | 1.00 | 38.79 |
| ATOM | 5749 | OH | TYR | 730 | 37.974 | -0.542 | 24.575 | 1.00 | 40.32 |
| ATOM | 5751 | C | TYR | 730 | 42.806 | -3.866 | 26.856 | 1.00 | 44.45 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5752 | O | TYR | 730 | 42.786 | -2.632 | 26.818 | 1.00 | 43.45 |
| ATOM | 5753 | N | MET | 731 | 42.798 | -4.534 | 28.006 | 1.00 | 46.44 |
| ATOM | 5755 | CA | MET | 731 | 42.805 | -3.812 | 29.279 | 1.00 | 48.59 |
| ATOM | 5756 | CB | MET | 731 | 42.516 | -4.748 | 30.447 | 1.00 | 54.69 |
| ATOM | 5757 | CG | MET | 731 | 41.132 | -5.387 | 30.398 | 1.00 | 62.68 |
| ATOM | 5758 | SD | MET | 731 | 39.781 | -4.189 | 30.392 | 1.00 | 70.49 |
| ATOM | 5759 | CE | MET | 731 | 39.492 | -4.012 | 32.209 | 1.00 | 72.27 |
| ATOM | 5760 | C | MET | 731 | 44.167 | -3.139 | 29.450 | 1.00 | 46.48 |
| ATOM | 5761 | O | MET | 731 | 44.280 | -2.085 | 30.086 | 1.00 | 44.91 |
| ATOM | 5762 | N | MET | 732 | 45.202 | -3.751 | 28.881 | 1.00 | 43.80 |
| ATOM | 5764 | CA | MET | 732 | 46.538 | -3.167 | 28.939 | 1.00 | 43.03 |
| ATOM | 5765 | CB | MET | 732 | 47.593 | -4.104 | 28.322 | 1.00 | 39.44 |
| ATOM | 5766 | CG | MET | 732 | 49.028 | -3.578 | 28.427 | 1.00 | 36.02 |
| ATOM | 5767 | SD | MET | 732 | 50.312 | -4.775 | 27.979 | 1.00 | 36.47 |
| ATOM | 5768 | CE | MET | 732 | 50.547 | -5.573 | 29.530 | 1.00 | 41.29 |
| ATOM | 5769 | C | MET | 732 | 46.474 | -1.833 | 28.188 | 1.00 | 42.08 |
| ATOM | 5770 | O | MET | 732 | 46.995 | -0.827 | 28.659 | 1.00 | 42.14 |
| ATOM | 5771 | N | MET | 733 | 45.775 | -1.822 | 27.054 | 1.00 | 43.14 |
| ATOM | 5773 | CA | MET | 733 | 45.608 | -0.609 | 26.257 | 1.00 | 42.24 |
| ATOM | 5774 | CB | MET | 733 | 44.852 | -0.877 | 24.947 | 1.00 | 41.41 |
| ATOM | 5775 | CG | MET | 733 | 45.607 | -1.730 | 23.938 | 1.00 | 40.23 |
| ATOM | 5776 | SD | MET | 733 | 44.669 | -2.025 | 22.419 | 1.00 | 38.02 |
| ATOM | 5777 | CE | MET | 733 | 45.183 | -3.724 | 21.982 | 1.00 | 28.12 |
| ATOM | 5778 | C | MET | 733 | 44.820 | 0.392 | 27.074 | 1.00 | 41.68 |
| ATOM | 5779 | O | MET | 733 | 45.215 | 1.550 | 27.196 | 1.00 | 43.78 |
| ATOM | 5780 | N | ARG | 734 | 43.713 | -0.053 | 27.655 | 1.00 | 42.59 |
| ATOM | 5782 | CA | ARG | 734 | 42.893 | 0.839 | 28.467 | 1.00 | 42.92 |
| ATOM | 5783 | CB | ARG | 734 | 41.642 | 0.119 | 28.966 | 1.00 | 42.35 |
| ATOM | 5784 | CG | ARG | 734 | 40.753 | -0.374 | 27.852 | 1.00 | 39.76 |
| ATOM | 5785 | CD | ARG | 734 | 40.360 | 0.763 | 26.959 | 1.00 | 41.83 |
| ATOM | 5786 | NE | ARG | 734 | 39.535 | 1.745 | 27.653 | 1.00 | 45.36 |
| ATOM | 5788 | CZ | ARG | 734 | 38.207 | 1.693 | 27.708 | 1.00 | 50.22 |
| ATOM | 5789 | NH1 | ARG | 734 | 37.542 | 0.708 | 27.117 | 1.00 | 51.18 |
| ATOM | 5792 | NH2 | ARG | 734 | 37.534 | 2.642 | 28.346 | 1.00 | 53.24 |
| ATOM | 5795 | C | ARG | 734 | 43.719 | 1.385 | 29.630 | 1.00 | 42.42 |
| ATOM | 5796 | O | ARG | 734 | 43.610 | 2.571 | 29.969 | 1.00 | 42.59 |
| ATOM | 5797 | N | ASP | 735 | 44.591 | 0.544 | 30.187 | 1.00 | 41.40 |
| ATOM | 5799 | CA | ASP | 735 | 45.464 | 0.959 | 31.286 | 1.00 | 43.33 |
| ATOM | 5800 | CB | ASP | 735 | 46.337 | -0.194 | 31.755 | 1.00 | 48.28 |
| ATOM | 5801 | CG | ASP | 735 | 45.556 | -1.256 | 32.496 | 1.00 | 54.86 |
| ATOM | 5802 | OD1 | ASP | 735 | 45.903 | -2.451 | 32.322 | 1.00 | 53.49 |
| ATOM | 5803 | OD2 | ASP | 735 | 44.612 | -0.900 | 33.245 | 1.00 | 55.59 |
| ATOM | 5804 | C | ASP | 735 | 46.365 | 2.107 | 30.840 | 1.00 | 42.65 |
| ATOM | 5805 | O | ASP | 735 | 46.484 | 3.124 | 31.543 | 1.00 | 44.03 |
| ATOM | 5806 | N | CYS | 736 | 47.021 | 1.926 | 29.693 | 1.00 | 38.83 |
| ATOM | 5808 | CA | CYS | 736 | 47.896 | 2.952 | 29.140 | 1.00 | 35.90 |
| ATOM | 5809 | CB | CYS | 736 | 48.545 | 2.468 | 27.858 | 1.00 | 33.62 |
| ATOM | 5810 | SG | CYS | 736 | 49.634 | 1.087 | 28.104 | 1.00 | 33.92 |
| ATOM | 5811 | C | CYS | 736 | 47.100 | 4.208 | 28.855 | 1.00 | 35.96 |
| ATOM | 5812 | O | CYS | 736 | 47.651 | 5.309 | 28.830 | 1.00 | 35.59 |
| ATOM | 5813 | N | TRP | 737 | 45.793 | 4.039 | 28.668 | 1.00 | 38.02 |
| ATOM | 5815 | CA | TRP | 737 | 44.906 | 5.156 | 28.372 | 1.00 | 40.14 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5816 | CB | TRP | 737 | 43.910 | 4.766 | 27.274 | 1.00 | 40.93 |
| ATOM | 5817 | CG | TRP | 737 | 44.563 | 4.379 | 25.977 | 1.00 | 42.36 |
| ATOM | 5818 | CD2 | TRP | 737 | 44.018 | 3.518 | 24.969 | 1.00 | 43.84 |
| ATOM | 5819 | CE2 | TRP | 737 | 44.972 | 3.437 | 23.929 | 1.00 | 46.42 |
| ATOM | 5820 | CE3 | TRP | 737 | 42.817 | 2.806 | 24.845 | 1.00 | 42.43 |
| ATOM | 5821 | CD1 | TRP | 737 | 45.793 | 4.775 | 25.519 | 1.00 | 42.57 |
| ATOM | 5822 | NE1 | TRP | 737 | 46.043 | 4.214 | 24.292 | 1.00 | 44.22 |
| ATOM | 5824 | CZ2 | TRP | 737 | 44.756 | 2.666 | 22.773 | 1.00 | 44.97 |
| ATOM | 5825 | CZ3 | TRP | 737 | 42.606 | 2.042 | 23.699 | 1.00 | 40.74 |
| ATOM | 5826 | CH2 | TRP | 737 | 43.571 | 1.978 | 22.682 | 1.00 | 40.75 |
| ATOM | 5827 | C | TRP | 737 | 44.157 | 5.706 | 29.584 | 1.00 | 40.62 |
| ATOM | 5828 | O | TRP | 737 | 43.085 | 6.285 | 29.437 | 1.00 | 41.37 |
| ATOM | 5829 | N | HIS | 738 | 44.706 | 5.533 | 30.783 | 1.00 | 42.09 |
| ATOM | 5831 | CA | HIS | 738 | 44.044 | 6.059 | 31.966 | 1.00 | 43.78 |
| ATOM | 5832 | CB | HIS | 738 | 44.635 | 5.463 | 33.248 | 1.00 | 46.52 |
| ATOM | 5833 | CG | HIS | 738 | 43.878 | 5.844 | 34.486 | 1.00 | 52.24 |
| ATOM | 5834 | CD2 | HIS | 738 | 43.599 | 7.053 | 35.025 | 1.00 | 50.95 |
| ATOM | 5835 | ND1 | HIS | 738 | 43.271 | 4.914 | 35.299 | 1.00 | 56.16 |
| ATOM | 5837 | CE1 | HIS | 738 | 42.643 | 5.536 | 36.285 | 1.00 | 57.23 |
| ATOM | 5838 | NE2 | HIS | 738 | 42.827 | 6.835 | 36.141 | 1.00 | 53.22 |
| ATOM | 5840 | C | HIS | 738 | 44.183 | 7.577 | 31.964 | 1.00 | 42.81 |
| ATOM | 5841 | O | HIS | 738 | 45.235 | 8.093 | 31.654 | 1.00 | 42.12 |
| ATOM | 5842 | N | ALA | 739 | 43.121 | 8.285 | 32.324 | 1.00 | 45.66 |
| ATOM | 5844 | CA | ALA | 739 | 43.130 | 9.750 | 32.350 | 1.00 | 49.42 |
| ATOM | 5845 | CB | ALA | 739 | 41.739 | 10.262 | 32.681 | 1.00 | 53.04 |
| ATOM | 5846 | C | ALA | 739 | 44.167 | 10.380 | 33.291 | 1.00 | 50.18 |
| ATOM | 5847 | O | ALA | 739 | 44.710 | 11.450 | 33.006 | 1.00 | 51.86 |
| ATOM | 5848 | N | VAL | 740 | 44.322 | 9.780 | 34.466 | 1.00 | 49.96 |
| ATOM | 5850 | CA | VAL | 740 | 45.299 | 10.219 | 35.467 | 1.00 | 50.17 |
| ATOM | 5851 | CB | VAL | 740 | 44.828 | 9.849 | 36.881 | 1.00 | 50.33 |
| ATOM | 5852 | CG1 | VAL | 740 | 45.880 | 10.209 | 37.896 | 1.00 | 51.40 |
| ATOM | 5853 | CG2 | VAL | 740 | 43.534 | 10.559 | 37.193 | 1.00 | 50.86 |
| ATOM | 5854 | C | VAL | 740 | 46.626 | 9.497 | 35.196 | 1.00 | 49.81 |
| ATOM | 5855 | O | VAL | 740 | 46.749 | 8.295 | 35.472 | 1.00 | 49.85 |
| ATOM | 5856 | N | PRO | 741 | 47.646 | 10.230 | 34.713 | 1.00 | 47.92 |
| ATOM | 5857 | CD | PRO | 741 | 47.618 | 11.683 | 34.476 | 1.00 | 46.97 |
| ATOM | 5858 | CA | PRO | 741 | 48.968 | 9.686 | 34.393 | 1.00 | 46.47 |
| ATOM | 5859 | CB | PRO | 741 | 49.796 | 10.941 | 34.134 | 1.00 | 44.38 |
| ATOM | 5860 | CG | PRO | 741 | 48.800 | 11.877 | 33.561 | 1.00 | 44.86 |
| ATOM | 5861 | C | PRO | 741 | 49.593 | 8.815 | 35.480 | 1.00 | 47.21 |
| ATOM | 5862 | O | PRO | 741 | 50.243 | 7.816 | 35.176 | 1.00 | 46.77 |
| ATOM | 5863 | N | SER | 742 | 49.380 | 9.181 | 36.741 | 1.00 | 48.87 |
| ATOM | 5865 | CA | SER | 742 | 49.939 | 8.430 | 37.860 | 1.00 | 50.19 |
| ATOM | 5866 | CB | SER | 742 | 49.753 | 9.203 | 39.166 | 1.00 | 51.87 |
| ATOM | 5867 | OG | SER | 742 | 48.389 | 9.514 | 39.391 | 1.00 | 54.19 |
| ATOM | 5869 | C | SER | 742 | 49.331 | 7.040 | 38.010 | 1.00 | 51.30 |
| ATOM | 5870 | O | SER | 742 | 49.863 | 6.192 | 38.723 | 1.00 | 51.14 |
| ATOM | 5871 | N | GLN | 743 | 48.207 | 6.814 | 37.343 | 1.00 | 53.07 |
| ATOM | 5873 | CA | GLN | 743 | 47.531 | 5.531 | 37.414 | 1.00 | 53.50 |
| ATOM | 5874 | CB | GLN | 743 | 46.015 | 5.745 | 37.548 | 1.00 | 59.34 |
| ATOM | 5875 | CG | GLN | 743 | 45.412 | 5.307 | 38.898 | 1.00 | 66.19 |
| ATOM | 5876 | CD | GLN | 743 | 46.133 | 5.896 | 40.106 | 1.00 | 70.07 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5877 | OE1 | GLN | 743 | 46.750 | 5.170 | 40.885 | 1.00 | 73.86 |
| ATOM | 5878 | NE2 | GLN | 743 | 46.047 | 7.209 | 40.273 | 1.00 | 72.01 |
| ATOM | 5881 | C | GLN | 743 | 47.850 | 4.613 | 36.236 | 1.00 | 51.14 |
| ATOM | 5882 | O | GLN | 743 | 47.504 | 3.425 | 36.266 | 1.00 | 51.79 |
| ATOM | 5883 | N | ARG | 744 | 48.484 | 5.153 | 35.196 | 1.00 | 48.31 |
| ATOM | 5885 | CA | ARG | 744 | 48.849 | 4.343 | 34.027 | 1.00 | 45.49 |
| ATOM | 5886 | CB | ARG | 744 | 49.326 | 5.224 | 32.869 | 1.00 | 40.33 |
| ATOM | 5887 | CG | ARG | 744 | 48.322 | 6.200 | 32.324 | 1.00 | 36.32 |
| ATOM | 5888 | CD | ARG | 744 | 48.944 | 7.100 | 31.262 | 1.00 | 28.55 |
| ATOM | 5889 | NE | ARG | 744 | 48.050 | 8.203 | 30.961 | 1.00 | 28.86 |
| ATOM | 5891 | CZ | ARG | 744 | 48.429 | 9.409 | 30.547 | 1.00 | 30.58 |
| ATOM | 5892 | NH1 | ARG | 744 | 49.707 | 9.700 | 30.357 | 1.00 | 26.02 |
| ATOM | 5895 | NH2 | ARG | 744 | 47.516 | 10.354 | 30.386 | 1.00 | 30.62 |
| ATOM | 5898 | C | ARG | 744 | 50.016 | 3.454 | 34.452 | 1.00 | 47.35 |
| ATOM | 5899 | O | ARG | 744 | 50.794 | 3.824 | 35.334 | 1.00 | 52.01 |
| ATOM | 5900 | N | PRO | 745 | 50.133 | 2.251 | 33.869 | 1.00 | 46.36 |
| ATOM | 5901 | CD | PRO | 745 | 49.248 | 1.559 | 32.921 | 1.00 | 45.54 |
| ATOM | 5902 | CA | PRO | 745 | 51.261 | 1.402 | 34.271 | 1.00 | 43.41 |
| ATOM | 5903 | CB | PRO | 745 | 50.972 | 0.078 | 33.547 | 1.00 | 41.77 |
| ATOM | 5904 | CG | PRO | 745 | 50.155 | 0.491 | 32.354 | 1.00 | 42.26 |
| ATOM | 5905 | C | PRO | 745 | 52.590 | 2.007 | 33.822 | 1.00 | 40.30 |
| ATOM | 5906 | O | PRO | 745 | 52.621 | 2.905 | 32.990 | 1.00 | 39.73 |
| ATOM | 5907 | N | THR | 746 | 53.679 | 1.570 | 34.433 | 1.00 | 39.14 |
| ATOM | 5909 | CA | THR | 746 | 54.997 | 2.056 | 34.039 | 1.00 | 38.35 |
| ATOM | 5910 | CB | THR | 746 | 55.992 | 2.104 | 35.249 | 1.00 | 36.75 |
| ATOM | 5911 | OG1 | THR | 746 | 56.202 | 0.776 | 35.769 | 1.00 | 32.25 |
| ATOM | 5913 | CG2 | THR | 746 | 55.477 | 3.037 | 36.341 | 1.00 | 30.31 |
| ATOM | 5914 | C | THR | 746 | 55.568 | 1.102 | 32.987 | 1.00 | 37.90 |
| ATOM | 5915 | O | THR | 746 | 55.185 | -0.068 | 32.938 | 1.00 | 37.99 |
| ATOM | 5916 | N | PHE | 747 | 56.490 | 1.584 | 32.157 | 1.00 | 35.94 |
| ATOM | 5918 | CA | PHE | 747 | 57.106 | 0.716 | 31.161 | 1.00 | 35.00 |
| ATOM | 5919 | CB | PHE | 747 | 58.124 | 1.469 | 30.309 | 1.00 | 30.45 |
| ATOM | 5920 | CG | PHE | 747 | 57.512 | 2.174 | 29.142 | 1.00 | 27.61 |
| ATOM | 5921 | CD1 | PHE | 747 | 56.950 | 1.450 | 28.103 | 1.00 | 23.68 |
| ATOM | 5922 | CD2 | PHE | 747 | 57.468 | 3.556 | 29.094 | 1.00 | 27.97 |
| ATOM | 5923 | CE1 | PHE | 747 | 56.352 | 2.088 | 27.033 | 1.00 | 23.56 |
| ATOM | 5924 | CE2 | PHE | 747 | 56.869 | 4.209 | 28.027 | 1.00 | 26.92 |
| ATOM | 5925 | CZ | PHE | 747 | 56.312 | 3.470 | 26.995 | 1.00 | 26.21 |
| ATOM | 5926 | C | PHE | 747 | 57.766 | -0.477 | 31.826 | 1.00 | 36.37 |
| ATOM | 5927 | O | PHE | 747 | 57.920 | -1.525 | 31.219 | 1.00 | 37.11 |
| ATOM | 5928 | N | LYS | 748 | 58.177 | -0.312 | 33.075 | 1.00 | 39.68 |
| ATOM | 5930 | CA | LYS | 748 | 58.797 | -1.411 | 33.807 | 1.00 | 42.20 |
| ATOM | 5931 | CB | LYS | 748 | 59.433 | -0.895 | 35.095 | 1.00 | 46.17 |
| ATOM | 5932 | CG | LYS | 748 | 59.978 | -1.991 | 35.984 | 1.00 | 54.78 |
| ATOM | 5933 | CD | LYS | 748 | 60.794 | -1.428 | 37.135 | 1.00 | 58.53 |
| ATOM | 5934 | CE | LYS | 748 | 61.239 | -2.537 | 38.075 | 1.00 | 59.33 |
| ATOM | 5935 | NZ | LYS | 748 | 62.167 | -2.025 | 39.120 | 1.00 | 62.36 |
| ATOM | 5939 | C | LYS | 748 | 57.723 | -2.463 | 34.111 | 1.00 | 42.78 |
| ATOM | 5940 | O | LYS | 748 | 57.998 | -3.664 | 34.075 | 1.00 | 37.97 |
| ATOM | 5941 | N | GLN | 749 | 56.503 | -1.992 | 34.392 | 1.00 | 43.27 |
| ATOM | 5943 | CA | GLN | 749 | 55.365 | -2.866 | 34.671 | 1.00 | 43.39 |
| ATOM | 5944 | CB | GLN | 749 | 54.146 | -2.056 | 35.146 | 1.00 | 47.37 |

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ATOM   5945  CG  GLN   749      54.236  -1.504  36.569  1.00 51.86
ATOM   5946  CD  GLN   749      53.036  -0.639  36.938  1.00 54.76
ATOM   5947  OE1 GLN   749      53.181   0.504  37.350  1.00 58.36
ATOM   5948  NE2 GLN   749      51.846  -1.179  36.769  1.00 59.25
ATOM   5951  C   GLN   749      55.006  -3.607  33.389  1.00 41.66
ATOM   5952  O   GLN   749      54.978  -4.841  33.355  1.00 40.25
ATOM   5953  N   LEU   750      54.759  -2.843  32.327  1.00 41.47
ATOM   5955  CA  LEU   750      54.398  -3.387  31.018  1.00 40.00
ATOM   5956  CB  LEU   750      54.366  -2.279  29.966  1.00 40.55
ATOM   5957  CG  LEU   750      53.316  -1.174  30.112  1.00 39.94
ATOM   5958  CD1 LEU   750      53.714   0.019  29.257  1.00 41.03
ATOM   5959  CD2 LEU   750      51.952  -1.696  29.722  1.00 37.80
ATOM   5960  C   LEU   750      55.383  -4.452  30.581  1.00 39.61
ATOM   5961  O   LEU   750      54.990  -5.470  30.027  1.00 42.08
ATOM   5962  N   VAL   751      56.670  -4.207  30.804  1.00 40.63
ATOM   5964  CA  VAL   751      57.691  -5.177  30.422  1.00 39.65
ATOM   5965  CB  VAL   751      59.115  -4.639  30.677  1.00 33.44
ATOM   5966  CG1 VAL   751      60.142  -5.694  30.351  1.00 31.57
ATOM   5967  CG2 VAL   751      59.372  -3.433  29.825  1.00 25.19
ATOM   5968  C   VAL   751      57.458  -6.468  31.204  1.00 43.58
ATOM   5969  O   VAL   751      57.530  -7.563  30.646  1.00 44.81
ATOM   5970  N   GLU   752      57.116  -6.339  32.481  1.00 46.24
ATOM   5972  CA  GLU   752      56.869  -7.518  33.301  1.00 50.55
ATOM   5973  CB  GLU   752      56.781  -7.137  34.783  1.00 53.70
ATOM   5974  CG  GLU   752      58.090  -6.541  35.310  1.00 56.60
ATOM   5975  CD  GLU   752      58.079  -6.243  36.792  1.00 56.20
ATOM   5976  OE1 GLU   752      58.387  -5.092  37.178  1.00 53.45
ATOM   5977  OE2 GLU   752      57.789  -7.170  37.573  1.00 60.28
ATOM   5978  C   GLU   752      55.622  -8.275  32.837  1.00 50.90
ATOM   5979  O   GLU   752      55.689  -9.474  32.555  1.00 51.03
ATOM   5980  N   ASP   753      54.501  -7.570  32.708  1.00 51.12
ATOM   5982  CA  ASP   753      53.251  -8.184  32.265  1.00 48.76
ATOM   5983  CB  ASP   753      52.122  -7.160  32.249  1.00 51.11
ATOM   5984  CG  ASP   753      51.646  -6.805  33.636  1.00 54.97
ATOM   5985  OD1 ASP   753      51.592  -7.715  34.495  1.00 58.37
ATOM   5986  OD2 ASP   753      51.319  -5.618  33.864  1.00 56.38
ATOM   5987  C   ASP   753      53.381  -8.790  30.881  1.00 48.02
ATOM   5988  O   ASP   753      52.991  -9.935  30.672  1.00 48.32
ATOM   5989  N   LEU   754      53.925  -8.020  29.940  1.00 45.16
ATOM   5991  CA  LEU   754      54.111  -8.490  28.571  1.00 44.82
ATOM   5992  CB  LEU   754      54.696  -7.387  27.691  1.00 42.70
ATOM   5993  CG  LEU   754      53.736  -6.263  27.298  1.00 42.92
ATOM   5994  CD1 LEU   754      54.500  -5.236  26.495  1.00 41.44
ATOM   5995  CD2 LEU   754      52.537  -6.822  26.502  1.00 42.86
ATOM   5996  C   LEU   754      55.001  -9.716  28.529  1.00 46.00
ATOM   5997  O   LEU   754      54.815 -10.606  27.708  1.00 45.88
ATOM   5998  N   ASP   755      55.975  -9.752  29.424  1.00 47.37
ATOM   6000  CA  ASP   755      56.889 -10.873  29.516  1.00 48.88
ATOM   6001  CB  ASP   755      57.898 -10.584  30.628  1.00 49.89
ATOM   6002  CG  ASP   755      58.998 -11.616  30.717  1.00 51.73
ATOM   6003  OD1 ASP   755      59.640 -11.680  31.785  1.00 55.47
ATOM   6004  OD2 ASP   755      59.236 -12.354  29.738  1.00 50.98
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| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 6005 | C | ASP | 755 | 56.024 | -12.093 | 29.864 | 1.00 | 51.26 | |
| ATOM | 6006 | O | ASP | 755 | 56.021 | -13.107 | 29.155 | 1.00 | 50.49 | |
| ATOM | 6007 | N | ARG | 756 | 55.227 | -11.940 | 30.917 | 1.00 | 52.15 | |
| ATOM | 6009 | CA | ARG | 756 | 54.332 | -12.989 | 31.385 | 1.00 | 53.30 | |
| ATOM | 6010 | CB | ARG | 756 | 53.556 | -12.501 | 32.611 | 1.00 | 54.54 | |
| ATOM | 6011 | CG | ARG | 756 | 52.389 | -13.380 | 33.029 | 1.00 | 54.26 | |
| ATOM | 6012 | CD | ARG | 756 | 51.672 | -12.772 | 34.215 | 1.00 | 56.76 | |
| ATOM | 6013 | NE | ARG | 756 | 51.293 | -11.382 | 33.969 | 1.00 | 61.39 | |
| ATOM | 6015 | CZ | ARG | 756 | 50.259 | -11.002 | 33.221 | 1.00 | 62.60 | |
| ATOM | 6016 | NH1 | ARG | 756 | 49.487 | -11.909 | 32.642 | 1.00 | 61.18 | |
| ATOM | 6019 | NH2 | ARG | 756 | 49.986 | -9.711 | 33.064 | 1.00 | 63.72 | |
| ATOM | 6022 | C | ARG | 756 | 53.357 | -13.420 | 30.297 | 1.00 | 53.03 | |
| ATOM | 6023 | O | ARG | 756 | 53.243 | -14.607 | 30.000 | 1.00 | 54.82 | |
| ATOM | 6024 | N | ILE | 757 | 52.687 | -12.452 | 29.680 | 1.00 | 51.18 | |
| ATOM | 6026 | CA | ILE | 757 | 51.709 | -12.732 | 28.630 | 1.00 | 48.68 | |
| ATOM | 6027 | CB | ILE | 757 | 51.025 | -11.435 | 28.120 | 1.00 | 47.88 | |
| ATOM | 6028 | CG2 | ILE | 757 | 50.112 | -11.752 | 26.953 | 1.00 | 45.56 | |
| ATOM | 6029 | CG1 | ILE | 757 | 50.247 | -10.763 | 29.258 | 1.00 | 47.77 | |
| ATOM | 6030 | CD1 | ILE | 757 | 49.651 | -9.414 | 28.914 | 1.00 | 46.00 | |
| ATOM | 6031 | C | ILE | 757 | 52.314 | -13.482 | 27.449 | 1.00 | 48.30 | |
| ATOM | 6032 | O | ILE | 757 | 51.694 | -14.409 | 26.937 | 1.00 | 45.61 | |
| ATOM | 6033 | N | VAL | 758 | 53.523 | -13.094 | 27.038 | 1.00 | 48.88 | |
| ATOM | 6035 | CA | VAL | 758 | 54.202 | -13.734 | 25.912 | 1.00 | 49.96 | |
| ATOM | 6036 | CB | VAL | 758 | 55.602 | -13.101 | 25.615 | 1.00 | 47.80 | |
| ATOM | 6037 | CG1 | VAL | 758 | 56.313 | -13.864 | 24.502 | 1.00 | 44.17 | |
| ATOM | 6038 | CG2 | VAL | 758 | 55.461 | -11.660 | 25.188 | 1.00 | 46.65 | |
| ATOM | 6039 | C | VAL | 758 | 54.378 | -15.217 | 26.196 | 1.00 | 54.00 | |
| ATOM | 6040 | O | VAL | 758 | 54.218 | -16.050 | 25.306 | 1.00 | 53.52 | |
| ATOM | 6041 | N | ALA | 759 | 54.697 | -15.540 | 27.445 | 1.00 | 57.83 | |
| ATOM | 6043 | CA | ALA | 759 | 54.898 | -16.926 | 27.844 | 1.00 | 61.94 | |
| ATOM | 6044 | CB | ALA | 759 | 55.447 | -16.987 | 29.257 | 1.00 | 62.30 | |
| ATOM | 6045 | C | ALA | 759 | 53.592 | -17.702 | 27.761 | 1.00 | 65.09 | |
| ATOM | 6046 | O | ALA | 759 | 53.555 | -18.823 | 27.254 | 1.00 | 66.39 | |
| ATOM | 6047 | N | LEU | 760 | 52.519 | -17.090 | 28.248 | 1.00 | 66.99 | |
| ATOM | 6049 | CA | LEU | 760 | 51.209 | -17.720 | 28.246 | 1.00 | 68.78 | |
| ATOM | 6050 | CB | LEU | 760 | 50.314 | -17.090 | 29.320 | 1.00 | 68.07 | |
| ATOM | 6051 | CG | LEU | 760 | 50.729 | -17.330 | 30.777 | 1.00 | 67.01 | |
| ATOM | 6052 | CD1 | LEU | 760 | 49.808 | -16.563 | 31.722 | 1.00 | 67.93 | |
| ATOM | 6053 | CD2 | LEU | 760 | 50.701 | -18.819 | 31.083 | 1.00 | 65.17 | |
| ATOM | 6054 | C | LEU | 760 | 50.510 | -17.666 | 26.892 | 1.00 | 71.19 | |
| ATOM | 6055 | O | LEU | 760 | 49.342 | -18.039 | 26.787 | 1.00 | 73.15 | |
| ATOM | 6056 | N | THR | 761 | 51.210 | -17.201 | 25.860 | 1.00 | 73.38 | |
| ATOM | 6058 | CA | THR | 761 | 50.626 | -17.113 | 24.518 | 1.00 | 73.92 | |
| ATOM | 6059 | CB | THR | 761 | 50.963 | -15.760 | 23.829 | 1.00 | 72.65 | |
| ATOM | 6060 | OG1 | THR | 761 | 50.353 | -14.690 | 24.555 | 1.00 | 74.44 | |
| ATOM | 6062 | CG2 | THR | 761 | 50.435 | -15.731 | 22.420 | 1.00 | 70.32 | |
| ATOM | 6063 | C | THR | 761 | 51.080 | -18.276 | 23.636 | 1.00 | 74.66 | |
| ATOM | 6064 | O | THR | 761 | 52.276 | -18.520 | 23.463 | 1.00 | 75.08 | |
| ATOM | 6065 | SG | CYS | 1603 | 19.100 | -9.073 | 19.903 | 0.50 | 30.84 | PRT2 |
| ATOM | 6066 | CG | MET | 534 | 69.385 | 12.295 | 23.393 | 0.50 | 33.69 | PRT2 |
| ATOM | 6067 | SD | MET | 534 | 69.112 | 13.312 | 24.832 | 0.50 | 34.44 | PRT2 |
| ATOM | 6068 | CE | MET | 534 | 70.067 | 12.429 | 26.060 | 0.50 | 36.92 | PRT2 |

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ATOM   6069  SG  CYS   603      56.370  -7.959  16.451  0.50 41.20  PRT2
ATOM   2716  OH2 TIP3    1      71.864  25.128   2.721  1.00 26.20
ATOM   2719  OH2 TIP3    2      39.862   4.160  16.115  1.00 42.43
ATOM   2722  OH2 TIP3    3      83.875  19.969  10.572  1.00 23.41
ATOM   2725  OH2 TIP3    4      83.585  20.356   7.953  1.00 30.15
ATOM   2728  OH2 TIP3    5      75.100  16.407   6.948  1.00 46.78
ATOM   2731  OH2 TIP3    6      86.616  19.701   9.707  1.00 44.37
ATOM   2734  OH2 TIP3    7      52.270  10.726  24.472  1.00 40.13
ATOM   2737  OH2 TIP3    8      55.346   9.394  22.489  1.00 29.09
ATOM   2740  OH2 TIP3    9      56.794   4.380  32.527  1.00 28.02
ATOM   2743  OH2 TIP3   10      52.425   4.653  13.421  1.00 18.63
ATOM   2746  OH2 TIP3   11      41.527   5.347  22.682  1.00 32.60
ATOM   2749  OH2 TIP3   12      44.868   9.058  21.659  1.00 34.90
ATOM   2752  OH2 TIP3   13      64.548  -2.881  29.048  1.00 32.56
ATOM   2755  OH2 TIP3   14      77.179  13.205  23.892  1.00 30.36
ATOM   2758  OH2 TIP3   15      79.309  16.826  18.132  1.00 55.69
ATOM   2761  OH2 TIP3   16      83.279  11.681  16.069  1.00 21.18
ATOM   2764  OH2 TIP3   17      13.978  -9.614   0.374  1.00 23.81
ATOM   2767  OH2 TIP3   18      38.294   0.616   5.237  1.00 48.89
ATOM   2770  OH2 TIP3   19      27.114   6.248   5.051  1.00 19.82
ATOM   2773  OH2 TIP3   20      34.369  -1.759  16.798  1.00 43.83
ATOM   2776  OH2 TIP3   21      20.500   2.296  28.237  1.00 53.46
ATOM   2779  OH2 TIP3   22      50.938 -11.733  38.257  1.00 51.73
ATOM   2782  OH2 TIP3   23      17.066  -5.917  -2.027  1.00 29.88
ATOM   2785  OH2 TIP3   24      27.873   8.078  15.136  1.00 46.40
ATOM   2788  OH2 TIP3   25      31.459   0.037   6.873  1.00 33.38
ATOM   2791  OH2 TIP3   26      27.088 -12.845  27.724  1.00 37.01
ATOM   2794  OH2 TIP3   27      28.577 -17.329  12.884  1.00 37.31
ATOM   2797  OH2 TIP3   28      88.863  14.111   8.054  1.00 41.25
ATOM   2800  OH2 TIP3   29      -2.311  -3.712  11.489  1.00 30.72
ATOM   2803  OH2 TIP3   30      34.895  -4.269  18.658  1.00 28.99
ATOM   2806  OH2 TIP3   31      80.531  18.007   9.739  1.00 23.83
ATOM   2809  OH2 TIP3   32       5.519   3.787  10.628  1.00 20.39
ATOM   2812  OH2 TIP3   33     -10.523   5.304  11.469  1.00 20.31
ATOM   2815  OH2 TIP3   34      29.538  -8.848  20.187  1.00 43.26
ATOM   2818  OH2 TIP3   35       5.866   3.469  13.367  1.00 21.16
ATOM   2821  OH2 TIP3   36      31.810   3.038   0.203  1.00 65.03
ATOM   2824  OH2 TIP3   37      19.879   2.087  -3.828  1.00 34.62
ATOM   2827  OH2 TIP3   38      61.882   2.577  32.790  1.00 43.01
ATOM   2830  OH2 TIP3   39      21.062  -6.897  -4.255  1.00 26.18
ATOM   2833  OH2 TIP3   40     -15.562   8.847  22.744  1.00 40.33
ATOM   2836  OH2 TIP3   41      40.043   2.380   8.610  1.00 65.14
ATOM   2839  OH2 TIP3   42      19.176  11.322   0.332  1.00 33.04
ATOM   2842  OH2 TIP3   43      67.221   8.965  17.535  1.00 14.78
ATOM   2845  OH2 TIP3   44      87.877  18.828  18.789  1.00 50.00
ATOM   2848  OH2 TIP3   45      74.676  17.083   4.253  1.00 43.45
ATOM   2851  OH2 TIP3   46      29.458  16.709  10.527  1.00 37.44
ATOM   2854  OH2 TIP3   47      66.590   7.242  15.359  1.00 27.63
ATOM   2857  OH2 TIP3   48      85.038  21.651   5.881  1.00 27.12
ATOM   2860  OH2 TIP3   49      -4.762   3.091   3.313  1.00 13.83
ATOM   2863  OH2 TIP3   50      19.509   4.951   5.063  1.00 33.74
ATOM   2866  OH2 TIP3   51      34.833   5.465  24.635  1.00 32.77
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| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2869 | OH2 | TIP3 | 52 | 34.907 | -17.187 | 13.739 | 1.00 | 39.47 |
| ATOM | 2872 | OH2 | TIP3 | 53 | 60.000 | 7.568 | 27.982 | 1.00 | 31.38 |
| ATOM | 2875 | OH2 | TIP3 | 54 | -7.341 | -1.418 | 6.308 | 1.00 | 40.22 |
| ATOM | 2878 | OH2 | TIP3 | 55 | 55.218 | 12.161 | 25.430 | 1.00 | 40.99 |
| ATOM | 2881 | OH2 | TIP3 | 56 | 68.597 | 6.912 | 16.955 | 1.00 | 45.39 |
| ATOM | 2884 | OH2 | TIP3 | 57 | 73.486 | 20.957 | 19.260 | 1.00 | 49.23 |
| ATOM | 2887 | OH2 | TIP3 | 58 | 3.555 | -8.367 | -8.166 | 1.00 | 20.02 |
| ATOM | 2890 | OH2 | TIP3 | 59 | 38.079 | 10.933 | 5.669 | 1.00 | 27.07 |
| ATOM | 2893 | OH2 | TIP3 | 60 | 29.817 | -9.690 | -1.649 | 1.00 | 44.28 |
| ATOM | 2896 | OH2 | TIP3 | 61 | 49.332 | 1.501 | 12.262 | 1.00 | 42.78 |
| ATOM | 2899 | OH2 | TIP3 | 62 | 41.366 | 3.969 | 28.834 | 1.00 | 37.60 |
| ATOM | 2902 | OH2 | TIP3 | 63 | 10.523 | -13.468 | 0.864 | 1.00 | 45.18 |
| ATOM | 2905 | OH2 | TIP3 | 64 | -1.001 | -4.658 | 21.574 | 1.00 | 35.58 |
| ATOM | 2908 | OH2 | TIP3 | 65 | 30.278 | 16.435 | 13.217 | 1.00 | 48.75 |
| ATOM | 2911 | OH2 | TIP3 | 66 | 8.115 | 4.304 | 3.317 | 1.00 | 16.04 |
| ATOM | 2914 | OH2 | TIP3 | 67 | 73.460 | 18.707 | 22.744 | 1.00 | 34.79 |
| ATOM | 2917 | OH2 | TIP3 | 68 | -8.041 | -3.332 | 24.939 | 1.00 | 44.96 |
| ATOM | 2920 | OH2 | TIP3 | 69 | 66.672 | -4.643 | 28.739 | 1.00 | 62.39 |
| ATOM | 2923 | OH2 | TIP3 | 70 | 21.770 | -20.943 | 4.990 | 1.00 | 32.98 |
| ATOM | 2926 | OH2 | TIP3 | 71 | 59.587 | -6.482 | 5.018 | 1.00 | 37.78 |
| ATOM | 2929 | OH2 | TIP3 | 72 | 16.676 | -13.158 | -3.023 | 1.00 | 42.74 |
| ATOM | 2932 | OH2 | TIP3 | 73 | -15.177 | 7.529 | 4.524 | 1.00 | 19.90 |
| ATOM | 2935 | OH2 | TIP3 | 74 | 33.105 | 2.738 | 13.267 | 1.00 | 40.43 |
| ATOM | 2938 | OH2 | TIP3 | 75 | 0.334 | -2.795 | 10.999 | 1.00 | 31.20 |
| ATOM | 2941 | OH2 | TIP3 | 76 | 17.489 | 2.568 | 5.445 | 1.00 | 16.38 |
| ATOM | 2944 | OH2 | TIP3 | 77 | 27.373 | 3.870 | 6.168 | 1.00 | 39.52 |
| ATOM | 2947 | OH2 | TIP3 | 78 | -8.546 | 6.378 | 9.673 | 1.00 | 17.89 |
| ATOM | 2950 | OH2 | TIP3 | 79 | 1.508 | -1.891 | 8.809 | 1.00 | 33.71 |
| ATOM | 2953 | OH2 | TIP3 | 80 | -4.985 | -3.024 | 6.965 | 1.00 | 29.65 |
| ATOM | 2956 | OH2 | TIP3 | 81 | 17.673 | 3.019 | 1.736 | 1.00 | 22.73 |
| ATOM | 2959 | OH2 | TIP3 | 82 | 20.319 | 3.536 | 2.883 | 1.00 | 20.39 |
| ATOM | 2962 | OH2 | TIP3 | 83 | 0.366 | -2.419 | 22.243 | 1.00 | 22.15 |
| ATOM | 2965 | OH2 | TIP3 | 84 | 19.688 | -6.134 | -1.678 | 1.00 | 13.22 |
| ATOM | 2968 | OH2 | TIP3 | 85 | 10.581 | -15.481 | 6.681 | 1.00 | 43.14 |
| ATOM | 2971 | OH2 | TIP3 | 86 | 4.476 | -12.368 | 11.861 | 1.00 | 38.38 |
| ATOM | 2974 | OH2 | TIP3 | 87 | 6.421 | 1.053 | -3.368 | 1.00 | 21.50 |
| ATOM | 2977 | OH2 | TIP3 | 88 | -13.766 | 1.683 | 5.565 | 1.00 | 39.45 |
| ATOM | 2980 | OH2 | TIP3 | 89 | 15.689 | -7.291 | -0.140 | 1.00 | 30.27 |
| ATOM | 2983 | OH2 | TIP3 | 90 | -1.762 | -5.389 | 3.937 | 1.00 | 31.03 |
| ATOM | 2986 | OH2 | TIP3 | 91 | 12.642 | 5.184 | -4.424 | 1.00 | 37.94 |
| ATOM | 2989 | OH2 | TIP3 | 92 | 69.601 | 27.513 | 2.309 | 1.00 | 44.71 |
| ATOM | 2992 | OH2 | TIP3 | 93 | 24.342 | -13.465 | -0.010 | 1.00 | 50.74 |
| ATOM | 2995 | OH2 | TIP3 | 94 | 60.354 | -4.675 | 33.978 | 1.00 | 38.15 |
| ATOM | 2998 | OH2 | TIP3 | 95 | 10.408 | 5.632 | 3.428 | 1.00 | 51.37 |
| ATOM | 3001 | OH2 | TIP3 | 96 | -9.676 | -3.916 | 4.621 | 1.00 | 34.12 |
| ATOM | 3004 | OH2 | TIP3 | 97 | 73.207 | -2.076 | 10.677 | 1.00 | 70.04 |
| ATOM | 3007 | OH2 | TIP3 | 98 | -3.042 | 5.487 | 30.579 | 1.00 | 30.78 |
| ATOM | 3010 | OH2 | TIP3 | 99 | 36.627 | 0.829 | 11.645 | 1.00 | 41.40 |
| ATOM | 3013 | OH2 | TIP3 | 100 | 21.685 | 6.318 | 16.814 | 1.00 | 20.93 |
| ATOM | 3016 | OH2 | TIP3 | 101 | 31.434 | 0.662 | 19.231 | 1.00 | 57.99 |
| ATOM | 3019 | OH2 | TIP3 | 102 | 5.793 | -8.713 | 22.177 | 1.00 | 54.77 |
| ATOM | 3022 | OH2 | TIP3 | 103 | -13.037 | 8.412 | 17.695 | 1.00 | 25.61 |

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ATOM    3025  OH2  TIP3   104       26.597 -10.647   -1.184   1.00 25.85
ATOM    3028  OH2  TIP3   105       24.406   1.951   18.037   1.00 30.72
ATOM    3031  OH2  TIP3   106       -1.809  12.914    3.754   1.00 43.57
ATOM    3034  OH2  TIP3   107       59.590  13.738   33.131   1.00 26.96
ATOM    3037  OH2  TIP3   108        4.442 -11.011    1.724   1.00 46.96
ATOM    3040  OH2  TIP3   109        8.101   2.869    0.801   1.00 37.28
ATOM    3043  OH2  TIP3   110       76.065   1.631   26.158   1.00 46.49
ATOM    3046  OH2  TIP3   111       48.821  15.839   14.239   1.00 34.18
ATOM    3049  OH2  TIP3   112        2.703 -11.324    8.959   1.00 39.16
ATOM    3052  OH2  TIP3   113       82.922  26.478   12.953   1.00 43.77
ATOM    3055  OH2  TIP3   114        8.998  -6.359   -3.309   1.00 39.51
ATOM    3058  OH2  TIP3   115       -8.590   4.563    4.397   1.00 32.53
ATOM    3061  OH2  TIP3   116        8.115 -13.800    8.351   1.00 41.64
ATOM    3064  OH2  TIP3   117       51.643   6.187   10.821   1.00 31.70
ATOM    3067  OH2  TIP3   118       20.737   3.915   15.522   1.00 17.40
ATOM    3070  OH2  TIP3   119       73.254   3.698   20.947   1.00 27.49
ATOM    3073  OH2  TIP3   120        5.343 -11.780   22.588   1.00 36.63
ATOM    3076  OH2  TIP3   121       34.390   2.307   16.660   1.00 64.04
ATOM    3079  OH2  TIP3   122        9.552 -11.846    6.934   1.00 28.23
ATOM    3082  OH2  TIP3   123        8.463   4.098   -1.454   1.00 30.21
ATOM    3085  OH2  TIP3   124        7.397   6.952    2.826   1.00 33.87
ATOM    3088  OH2  TIP3   125       35.796  -1.428    0.072   1.00 30.27
ATOM    3091  OH2  TIP3   126       45.044  10.052   11.102   1.00 28.75
ATOM    3094  OH2  TIP3   127       45.209  11.756   21.279   1.00 31.80
ATOM    3097  OH2  TIP3   128       -2.800  15.170   16.902   1.00 32.72
ATOM    3100  OH2  TIP3   129       85.885  11.248    9.428   1.00 25.28
ATOM    3103  OH2  TIP3   130       13.136  -2.420    1.867   1.00 20.56
ATOM    3106  OH2  TIP3   131       75.900   3.542   20.641   1.00 39.79
ATOM    3109  OH2  TIP3   132       13.075   7.580   -2.817   1.00 34.49
ATOM    3112  OH2  TIP3   133       11.166 -10.189    0.573   1.00 36.71
ATOM    3115  OH2  TIP3   134       13.814 -16.459    3.327   1.00 21.18
ATOM    3118  OH2  TIP3   135       -6.419  -3.460   16.599   1.00 32.62
ATOM    3121  OH2  TIP3   136       25.578 -12.834    3.624   1.00 43.32
ATOM    3124  OH2  TIP3   137      -16.472  11.136    6.388   1.00 64.77
ATOM    3127  OH2  TIP3   138       86.531  12.711    7.151   1.00 28.72
ATOM    3130  OH2  TIP3   139       32.292  -4.665    1.511   1.00 30.98
ATOM    3133  OH2  TIP3   140       45.116   7.369   11.774   1.00 30.59
ATOM    3136  OH2  TIP3   141       81.035  12.317   16.907   1.00 41.72
ATOM    3139  OH2  TIP3   142        2.905  -7.019   -2.101   1.00 26.20
ATOM    3142  OH2  TIP3   143       31.895  -6.253   20.885   1.00 36.12
ATOM    3145  OH2  TIP3   144       74.974  -2.640   12.464   1.00 58.90
ATOM    3148  OH2  TIP3   145        7.514   6.734   -1.116   1.00 37.81
ATOM    3151  OH2  TIP3   146       71.606   5.595   22.198   1.00 54.82
ATOM    3154  OH2  TIP3   147       68.337  -5.037    8.955   1.00 40.80
ATOM    3157  OH2  TIP3   148        0.191  -9.669    6.903   1.00 47.40
ATOM    3160  OH2  TIP3   149       68.043  18.153   10.710   1.00 36.67
ATOM    3163  OH2  TIP3   150        3.644   8.512    4.478   1.00 40.16
ATOM    3166  OH2  TIP3   151       52.117  11.302   18.644   1.00 40.22
ATOM    3169  OH2  TIP3   152      -10.220   6.750    4.981   1.00 25.00
ATOM    3172  OH2  TIP3   153       76.944   1.425   -0.793   1.00 46.95
ATOM    3175  OH2  TIP3   154       10.053 -11.958   17.014   1.00 38.99
ATOM    3178  OH2  TIP3   155       34.348  14.128   18.169   1.00 42.98
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| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3181 | OH2 | TIP3 | 156 | 2.472 | -8.230 | 16.629 | 1.00 | 39.28 |
| ATOM | 3184 | OH2 | TIP3 | 157 | 29.861 | 1.764 | 5.993 | 1.00 | 36.29 |
| ATOM | 3187 | OH2 | TIP3 | 158 | 32.608 | -17.351 | 11.473 | 1.00 | 59.48 |
| ATOM | 3190 | OH2 | TIP3 | 159 | 42.408 | 18.047 | 11.188 | 1.00 | 39.61 |
| ATOM | 3193 | OH2 | TIP3 | 160 | 88.019 | 10.498 | 5.885 | 1.00 | 57.85 |
| ATOM | 3196 | OH2 | TIP3 | 161 | 70.091 | -4.165 | 25.232 | 1.00 | 64.48 |
| ATOM | 3199 | OH2 | TIP3 | 162 | 77.332 | 5.434 | 24.000 | 1.00 | 55.68 |
| ATOM | 3202 | OH2 | TIP3 | 163 | -0.743 | -8.232 | 4.456 | 1.00 | 61.30 |
| ATOM | 3205 | OH2 | TIP3 | 164 | 34.224 | 15.617 | 1.556 | 1.00 | 36.76 |
| ATOM | 3208 | OH2 | TIP3 | 165 | -9.619 | 7.593 | 7.404 | 1.00 | 36.55 |
| ATOM | 3211 | OH2 | TIP3 | 166 | 11.725 | 5.841 | 7.590 | 1.00 | 33.56 |
| ATOM | 3214 | OH2 | TIP3 | 167 | -8.492 | 14.057 | 13.866 | 1.00 | 43.88 |
| ATOM | 3217 | OH2 | TIP3 | 168 | 32.082 | 3.374 | 18.430 | 1.00 | 50.87 |
| ATOM | 3220 | OH2 | TIP3 | 169 | -8.471 | 9.925 | 24.255 | 1.00 | 41.24 |
| ATOM | 3223 | OH2 | TIP3 | 170 | -1.100 | -6.507 | 15.528 | 1.00 | 31.24 |
| ATOM | 3226 | OH2 | TIP3 | 171 | 80.411 | 0.680 | 15.823 | 1.00 | 49.76 |
| ATOM | 3229 | OH2 | TIP3 | 172 | 67.266 | 20.862 | -1.548 | 1.00 | 43.71 |
| ATOM | 3232 | OH2 | TIP3 | 173 | -0.460 | 4.230 | 1.362 | 1.00 | 29.46 |
| ATOM | 3235 | OH2 | TIP3 | 174 | -0.107 | 6.721 | 2.716 | 1.00 | 34.57 |
| ATOM | 3238 | OH2 | TIP3 | 175 | -0.955 | 8.958 | 1.388 | 1.00 | 37.76 |
| ATOM | 3241 | OH2 | TIP3 | 176 | -5.269 | 9.229 | 2.243 | 1.00 | 38.77 |
| ATOM | 3244 | OH2 | TIP3 | 177 | -7.000 | 10.196 | 3.928 | 1.00 | 55.41 |
| ATOM | 3247 | OH2 | TIP3 | 178 | 2.919 | 7.005 | 0.987 | 1.00 | 46.54 |
| ATOM | 3250 | OH2 | TIP3 | 179 | 5.370 | 10.843 | 8.420 | 1.00 | 36.98 |
| ATOM | 3253 | OH2 | TIP3 | 180 | 63.828 | 12.793 | 22.770 | 1.00 | 63.91 |
| ATOM | 3256 | OH2 | TIP3 | 181 | 79.461 | 0.958 | 18.507 | 1.00 | 47.46 |
| ATOM | 3259 | OH2 | TIP3 | 182 | 59.131 | -11.907 | 7.222 | 1.00 | 51.47 |
| ATOM | 3262 | OH2 | TIP3 | 183 | 14.248 | -1.085 | -4.437 | 1.00 | 43.69 |
| ATOM | 3265 | OH2 | TIP3 | 184 | 59.294 | 2.993 | 33.283 | 1.00 | 56.42 |
| ATOM | 3268 | OH2 | TIP3 | 185 | 32.270 | 13.672 | 20.001 | 1.00 | 47.71 |
| ATOM | 3271 | OH2 | TIP3 | 186 | 72.089 | 16.139 | 22.904 | 1.00 | 49.99 |
| ATOM | 3274 | OH2 | TIP3 | 187 | 1.038 | -8.592 | 14.174 | 1.00 | 40.01 |
| ATOM | 3277 | OH2 | TIP3 | 188 | -0.484 | 5.267 | 30.679 | 1.00 | 48.08 |
| ATOM | 3280 | OH2 | TIP3 | 189 | 81.532 | 15.288 | 17.279 | 1.00 | 79.71 |
| ATOM | 3283 | OH2 | TIP3 | 190 | -17.528 | 3.859 | 24.112 | 1.00 | 56.21 |
| ATOM | 3286 | OH2 | TIP3 | 191 | 27.542 | 10.591 | 14.666 | 1.00 | 53.58 |
| ATOM | 3289 | OH2 | TIP3 | 192 | 34.962 | 4.381 | 27.739 | 1.00 | 60.92 |
| ATOM | 3292 | OH2 | TIP3 | 193 | -3.244 | -3.943 | 8.937 | 1.00 | 35.88 |
| ATOM | 3295 | OH2 | TIP3 | 194 | 42.673 | 7.836 | 22.289 | 1.00 | 37.44 |
| ATOM | 3298 | OH2 | TIP3 | 195 | 52.865 | 12.074 | 22.272 | 1.00 | 35.63 |
| ATOM | 3301 | OH2 | TIP3 | 196 | 26.791 | 13.926 | 19.808 | 1.00 | 76.14 |
| ATOM | 3304 | OH2 | TIP3 | 197 | -7.584 | 9.157 | 6.269 | 1.00 | 44.54 |
| ATOM | 3310 | OH2 | TIP3 | 198 | 55.298 | 15.955 | 20.455 | 1.00 | 50.69 |
| ATOM | 3313 | OH2 | TIP3 | 199 | 51.654 | 19.308 | 22.767 | 1.00 | 53.00 |
| ATOM | 3316 | OH2 | TIP3 | 200 | 20.092 | 7.039 | 7.056 | 1.00 | 32.98 |
| ATOM | 3319 | OH2 | TIP3 | 201 | 28.988 | 1.734 | -3.437 | 1.00 | 42.52 |
| ATOM | 3322 | OH2 | TIP3 | 202 | 26.359 | 2.749 | -4.689 | 1.00 | 43.12 |
| ATOM | 3325 | OH2 | TIP3 | 203 | 36.827 | 2.974 | 18.493 | 1.00 | 57.91 |
| ATOM | 3328 | OH2 | TIP3 | 204 | 17.012 | -20.743 | 13.983 | 1.00 | 62.01 |
| ATOM | 3331 | OH2 | TIP3 | 205 | 27.980 | -14.283 | 6.114 | 1.00 | 79.57 |
| ATOM | 3334 | OH2 | TIP3 | 206 | 31.396 | 1.595 | -1.941 | 1.00 | 53.29 |
| ATOM | 3337 | OH2 | TIP3 | 207 | 10.244 | -16.264 | 15.463 | 1.00 | 43.25 |

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ATOM    3340  OH2  TIP3   208        7.255 -11.909   5.440   1.00 45.52
ATOM    3343  OH2  TIP3   209      -12.421  14.520  11.103   1.00 56.32
ATOM    3346  OH2  TIP3   210       11.250   9.879  -1.498   1.00 28.34
ATOM    3349  OH2  TIP3   211       11.426  12.574  -1.341   1.00 37.79
ATOM    3352  OH2  TIP3   212       34.344  13.104  -1.291   1.00 51.83
ATOM    3355  OH2  TIP3   213       31.230  18.082   8.054   1.00 44.77
ATOM    3358  OH2  TIP3   214       37.062  12.036  -1.875   1.00 53.61
ATOM    3361  OH2  TIP3   215       35.231   3.150  10.692   1.00 60.59
ATOM    3364  OH2  TIP3   216       63.913  13.371  26.770   1.00 59.44
ATOM    3367  OH2  TIP3   217       36.511   6.165  15.409   1.00 70.98
ATOM    3370  OH2  TIP3   218       90.623   4.459   6.671   1.00 52.23
ATOM    3373  OH2  TIP3   219       49.822 -11.758  10.881   1.00 46.12
ATOM    3376  OH2  TIP3   220       60.367 -10.286  16.662   1.00 68.41
ATOM    3379  OH2  TIP3   221       17.954 -21.378   7.048   1.00 68.51
ATOM    3382  OH2  TIP3   222       66.176  -1.266  30.784   1.00 39.19
ATOM    3385  OH2  TIP3   223       75.201  19.402  20.800   1.00 43.98
ATOM    3388  OH2  TIP3   224       -2.895  10.302   3.534   1.00 44.97
ATOM    3391  OH2  TIP3   225        6.045  -4.015  25.279   1.00 63.74
ATOM    3394  OH2  TIP3   226       36.238   5.898  12.819   1.00 32.89
ATOM    3397  OH2  TIP3   227       -5.516  16.713  14.089   1.00 51.60
ATOM    3400  OH2  TIP3   228       46.577 -11.931  26.964   1.00 37.76
ATOM    3403  OH2  TIP3   229        6.496   6.048  13.722   1.00 27.51
ATOM    3406  OH2  TIP3   230       -3.691  -5.054  20.691   1.00 38.16
ATOM    3409  OH2  TIP3   231        1.811  -3.444  -0.149   1.00 54.03
ATOM    3412  OH2  TIP3   232       86.148  11.480  23.402   1.00 57.66
ATOM    3415  OH2  TIP3   233       10.549   7.581   5.716   1.00 48.49
ATOM    3421  OH2  TIP3   234       64.680  -8.130  20.697   1.00 69.67
ATOM    3424  OH2  TIP3   235       11.380 -17.736  13.500   1.00 54.61
ATOM    3427  OH2  TIP3   236        3.136  -4.782  21.980   1.00 57.12
ATOM    3430  OH2  TIP3   237       72.296   1.006  -1.987   1.00 41.40
ATOM    3433  OH2  TIP3   238       50.258  -3.179  32.723   1.00 74.99
ATOM    3436  OH2  TIP3   239       58.051   9.469  11.776   1.00 44.10
ATOM    3439  OH2  TIP3   240       43.530  20.498  30.344   1.00 43.69
ATOM    3442  OH2  TIP3   241       67.081  16.597  15.934   1.00 45.80
ATOM    3445  OH2  TIP3   242       87.660  21.694   5.373   1.00 50.39
ATOM    3448  OH2  TIP3   243       71.779  28.586   7.932   1.00 61.12
ATOM    3451  OH2  TIP3   244       25.965  -8.124  27.084   1.00 42.13
ATOM    3454  OH2  TIP3   245      -18.336  10.487  12.859   1.00 73.36
ATOM    3457  OH2  TIP3   246       30.703  11.410  16.381   1.00 39.24
ATOM    3460  OH2  TIP3   247       22.617 -16.025  -2.906   1.00 63.22
ATOM    4620  C    SUG   1000       67.815   4.441  11.493   1.00 20.00
ATOM    4621  C1   SUG   1000       67.387   3.706  10.364   1.00 20.00
ATOM    4622  N    SUG   1000       67.823   2.445   9.937   1.00 20.00
ATOM    4623  C2   SUG   1000       66.401   4.224   9.501   1.00 20.00
ATOM    4624  C3   SUG   1000       65.825   5.499   9.765   1.00 20.00
ATOM    4625  C4   SUG   1000       66.259   6.212  10.884   1.00 20.00
ATOM    4626  C5   SUG   1000       67.239   5.690  11.736   1.00 20.00
ATOM    4627  C6   SUG   1000       66.155   3.220   8.401   1.00 20.00
ATOM    4628  O    SUG   1000       67.372   1.047   8.275   1.00 20.00
ATOM    4629  C7   SUG   1000       67.155   2.121   8.828   1.00 20.00
ATOM    4630  C8   SUG   1000       63.369   2.460   5.852   1.00 20.00
ATOM    4631  C9   SUG   1000       65.284   3.356   7.382   1.00 20.00
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ATOM   4632  C10  SUG  1000     64.603   2.300   6.514  1.00 20.00
ATOM   4633  C11  SUG  1000     64.167   0.392   5.481  1.00 20.00
ATOM   4634  C12  SUG  1000     63.106   1.251   5.206  1.00 20.00
ATOM   4635  N13  SUG  1000     65.103   1.023   6.293  1.00 20.00
ATOM   4636  C14  SUG  1000     61.898   0.897   4.346  1.00 20.00
ATOM   4637  C15  SUG  1000     62.476   3.715   5.826  1.00 20.00
ATOM   4638  C16  SUG  1000     61.259   3.598   6.771  1.00 20.00
ATOM   4639  O1   SUG  1000     60.814   5.963   6.429  1.00 20.00
ATOM   4640  C17  SUG  1000     60.520   4.912   6.988  1.00 20.00
ATOM   4641  O2   SUG  1000     59.496   4.795   7.873  1.00 20.00
ATOM   4642  C    SUG  1001      5.413   2.967  18.087  1.00 20.00
ATOM   4643  C1   SUG  1001      5.891   2.927  19.417  1.00 20.00
ATOM   4644  N    SUG  1001      5.553   2.021  20.431  1.00 20.00
ATOM   4645  C2   SUG  1001      6.828   3.875  19.872  1.00 20.00
ATOM   4646  C3   SUG  1001      7.304   4.884  18.988  1.00 20.00
ATOM   4647  C4   SUG  1001      6.822   4.909  17.678  1.00 20.00
ATOM   4648  C5   SUG  1001      5.890   3.964  17.233  1.00 20.00
ATOM   4649  C6   SUG  1001      7.145   3.576  21.318  1.00 20.00
ATOM   4650  O    SUG  1001      6.101   1.678  22.552  1.00 20.00
ATOM   4651  C7   SUG  1001      6.237   2.343  21.530  1.00 20.00
ATOM   4652  C8   SUG  1001      9.967   4.392  23.809  1.00 20.00
ATOM   4653  C9   SUG  1001      7.997   4.264  22.102  1.00 20.00
ATOM   4654  C10  SUG  1001      8.753   3.835  23.357  1.00 20.00
ATOM   4655  C11  SUG  1001      9.331   2.736  25.189  1.00 20.00
ATOM   4656  C12  SUG  1001     10.320   3.689  24.962  1.00 20.00
ATOM   4657  N13  SUG  1001      8.354   2.808  24.203  1.00 20.00
ATOM   4658  C14  SUG  1001     11.547   3.900  25.843  1.00 20.00
ATOM   4659  C15  SUG  1001     10.759   5.550  23.175  1.00 20.00
ATOM   4660  C16  SUG  1001     11.987   5.063  22.373  1.00 20.00
ATOM   4661  O1   SUG  1001     12.243   7.308  21.475  1.00 20.00
ATOM   4662  C17  SUG  1001     12.621   6.142  21.504  1.00 20.00
ATOM   4663  O2   SUG  1001     13.657   5.670  20.762  1.00 20.00
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TABLE 4

| Atom No. | | Atom Type | A.A Type | A.A No. | X | Y | Z | OCC | B |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1 | N | GLU | 1464 | -13.576 | 17.066 | 8.598 | 1.00 | 57.39 |
| ATOM | 2 | CA | GLU | 1464 | -12.446 | 17.198 | 7.684 | 1.00 | 55.83 |
| ATOM | 3 | CB | GLU | 1464 | -11.381 | 18.127 | 8.275 | 1.00 | 56.73 |
| ATOM | 4 | C | GLU | 1464 | -11.845 | 15.833 | 7.341 | 1.00 | 55.07 |
| ATOM | 5 | O | GLU | 1464 | -11.722 | 15.504 | 6.165 | 1.00 | 59.74 |
| ATOM | 6 | N | LEU | 1465 | -11.518 | 15.023 | 8.347 | 1.00 | 50.12 |
| ATOM | 7 | CA | LEU | 1465 | -10.950 | 13.699 | 8.087 | 1.00 | 44.43 |
| ATOM | 8 | CB | LEU | 1465 | -10.155 | 13.196 | 9.291 | 1.00 | 43.28 |
| ATOM | 9 | CG | LEU | 1465 | -8.630 | 13.316 | 9.227 | 1.00 | 43.70 |
| ATOM | 10 | CD1 | LEU | 1465 | -8.222 | 14.754 | 9.013 | 1.00 | 47.59 |
| ATOM | 11 | CD2 | LEU | 1465 | -8.017 | 12.803 | 10.506 | 1.00 | 42.63 |
| ATOM | 12 | C | LEU | 1465 | -12.046 | 12.697 | 7.739 | 1.00 | 40.93 |
| ATOM | 13 | O | LEU | 1465 | -13.139 | 12.730 | 8.301 | 1.00 | 39.13 |
| ATOM | 14 | N | PRO | 1466 | -11.794 | 11.852 | 6.726 | 1.00 | 40.49 |
| ATOM | 15 | CD | PRO | 1466 | -10.612 | 11.884 | 5.844 | 1.00 | 39.07 |
| ATOM | 16 | CA | PRO | 1466 | -12.754 | 10.831 | 6.284 | 1.00 | 40.14 |
| ATOM | 17 | CB | PRO | 1466 | -12.152 | 10.331 | 4.981 | 1.00 | 40.90 |
| ATOM | 18 | CG | PRO | 1466 | -10.664 | 10.518 | 5.202 | 1.00 | 41.39 |
| ATOM | 19 | C | PRO | 1466 | -12.862 | 9.701 | 7.305 | 1.00 | 40.06 |
| ATOM | 20 | O | PRO | 1466 | -11.857 | 9.290 | 7.883 | 1.00 | 40.71 |
| ATOM | 21 | N | GLU | 1467 | -14.064 | 9.175 | 7.491 | 1.00 | 38.65 |
| ATOM | 22 | CA | GLU | 1467 | -14.255 | 8.126 | 8.467 | 1.00 | 39.24 |
| ATOM | 23 | CB | GLU | 1467 | -15.722 | 8.054 | 8.873 | 1.00 | 45.06 |
| ATOM | 24 | CG | GLU | 1467 | -16.314 | 9.365 | 9.353 | 1.00 | 50.91 |
| ATOM | 25 | CD | GLU | 1467 | -17.789 | 9.252 | 9.699 | 1.00 | 53.51 |
| ATOM | 26 | OE1 | GLU | 1467 | -18.379 | 8.170 | 9.504 | 1.00 | 54.15 |
| ATOM | 27 | OE2 | GLU | 1467 | -18.369 | 10.250 | 10.160 | 1.00 | 53.10 |
| ATOM | 28 | C | GLU | 1467 | -13.808 | 6.777 | 7.914 | 1.00 | 36.09 |
| ATOM | 29 | O | GLU | 1467 | -13.922 | 6.529 | 6.711 | 1.00 | 38.58 |
| ATOM | 30 | N | ASP | 1468 | -13.272 | 5.929 | 8.791 | 1.00 | 30.71 |
| ATOM | 31 | CA | ASP | 1468 | -12.839 | 4.592 | 8.407 | 1.00 | 28.23 |
| ATOM | 32 | CB | ASP | 1468 | -11.328 | 4.515 | 8.186 | 1.00 | 25.51 |
| ATOM | 33 | CG | ASP | 1468 | -10.885 | 3.207 | 7.529 | 1.00 | 27.68 |
| ATOM | 34 | OD1 | ASP | 1468 | -11.623 | 2.199 | 7.572 | 1.00 | 26.01 |
| ATOM | 35 | OD2 | ASP | 1468 | -9.777 | 3.187 | 6.962 | 1.00 | 28.87 |
| ATOM | 36 | C | ASP | 1468 | -13.274 | 3.627 | 9.493 | 1.00 | 27.74 |
| ATOM | 37 | O | ASP | 1468 | -12.570 | 3.405 | 10.493 | 1.00 | 25.83 |
| ATOM | 38 | N | PRO | 1469 | -14.450 | 3.019 | 9.305 | 1.00 | 25.88 |
| ATOM | 39 | CD | PRO | 1469 | -15.396 | 3.175 | 8.183 | 1.00 | 24.25 |
| ATOM | 40 | CA | PRO | 1469 | -14.963 | 2.079 | 10.294 | 1.00 | 26.69 |
| ATOM | 41 | CB | PRO | 1469 | -16.255 | 1.586 | 9.641 | 1.00 | 28.81 |
| ATOM | 42 | CG | PRO | 1469 | -16.702 | 2.776 | 8.816 | 1.00 | 24.20 |
| ATOM | 43 | C | PRO | 1469 | -14.012 | 0.925 | 10.625 | 1.00 | 27.51 |
| ATOM | 44 | O | PRO | 1469 | -14.172 | 0.285 | 11.657 | 1.00 | 27.60 |
| ATOM | 45 | N | ARG | 1470 | -13.075 | 0.642 | 9.720 | 1.00 | 26.49 |
| ATOM | 46 | CA | ARG | 1470 | -12.108 | -0.435 | 9.935 | 1.00 | 27.60 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 47 | CB | ARG | 1470 | -11.285 | -0.691 | 8.668 | 1.00 | 26.08 |
| ATOM | 48 | CG | ARG | 1470 | -12.073 | -1.125 | 7.439 | 1.00 | 30.77 |
| ATOM | 49 | CD | ARG | 1470 | -11.153 | -1.257 | 6.213 | 1.00 | 31.66 |
| ATOM | 50 | NE | ARG | 1470 | -10.462 | 0.001 | 5.915 | 1.00 | 30.94 |
| ATOM | 51 | CZ | ARG | 1470 | -9.577 | 0.167 | 4.941 | 1.00 | 33.30 |
| ATOM | 52 | NH1 | ARG | 1470 | -9.249 | -0.846 | 4.144 | 1.00 | 32.78 |
| ATOM | 53 | NH2 | ARG | 1470 | -8.990 | 1.346 | 4.779 | 1.00 | 27.16 |
| ATOM | 54 | C | ARG | 1470 | -11.116 | -0.163 | 11.069 | 1.00 | 28.73 |
| ATOM | 55 | O | ARG | 1470 | -10.588 | -1.091 | 11.673 | 1.00 | 27.30 |
| ATOM | 56 | N | TRP | 1471 | -10.871 | 1.107 | 11.363 | 1.00 | 27.98 |
| ATOM | 57 | CA | TRP | 1471 | -9.892 | 1.430 | 12.375 | 1.00 | 26.33 |
| ATOM | 58 | CB | TRP | 1471 | -8.642 | 1.964 | 11.671 | 1.00 | 23.87 |
| ATOM | 59 | CG | TRP | 1471 | -7.998 | 0.947 | 10.795 | 1.00 | 24.61 |
| ATOM | 60 | CD2 | TRP | 1471 | -7.110 | -0.104 | 11.205 | 1.00 | 23.32 |
| ATOM | 61 | CE2 | TRP | 1471 | -6.732 | -0.807 | 10.041 | 1.00 | 24.34 |
| ATOM | 62 | CE3 | TRP | 1471 | -6.589 | -0.509 | 12.438 | 1.00 | 21.39 |
| ATOM | 63 | CD1 | TRP | 1471 | -8.129 | 0.831 | 9.446 | 1.00 | 25.07 |
| ATOM | 64 | NE1 | TRP | 1471 | -7.369 | -0.220 | 8.980 | 1.00 | 26.82 |
| ATOM | 65 | CZ2 | TRP | 1471 | -5.860 | -1.898 | 10.083 | 1.00 | 23.12 |
| ATOM | 66 | CZ3 | TRP | 1471 | -5.722 | -1.589 | 12.473 | 1.00 | 21.02 |
| ATOM | 67 | CH2 | TRP | 1471 | -5.364 | -2.265 | 11.306 | 1.00 | 21.74 |
| ATOM | 68 | C | TRP | 1471 | -10.292 | 2.384 | 13.478 | 1.00 | 26.93 |
| ATOM | 69 | O | TRP | 1471 | -9.551 | 2.544 | 14.452 | 1.00 | 26.37 |
| ATOM | 70 | N | GLU | 1472 | -11.464 | 2.975 | 13.364 | 1.00 | 26.40 |
| ATOM | 71 | CA | GLU | 1472 | -11.909 | 3.959 | 14.341 | 1.00 | 27.12 |
| ATOM | 72 | CB | GLU | 1472 | -13.168 | 4.674 | 13.821 | 1.00 | 28.25 |
| ATOM | 73 | CG | GLU | 1472 | -13.497 | 6.026 | 14.498 | 1.00 | 27.47 |
| ATOM | 74 | CD | GLU | 1472 | -12.611 | 7.180 | 14.042 | 1.00 | 24.64 |
| ATOM | 75 | OE1 | GLU | 1472 | -11.877 | 7.038 | 13.042 | 1.00 | 24.60 |
| ATOM | 76 | OE2 | GLU | 1472 | -12.658 | 8.247 | 14.683 | 1.00 | 23.70 |
| ATOM | 77 | C | GLU | 1472 | -12.179 | 3.421 | 15.735 | 1.00 | 25.89 |
| ATOM | 78 | O | GLU | 1472 | -12.795 | 2.373 | 15.891 | 1.00 | 27.74 |
| ATOM | 79 | N | LEU | 1473 | -11.689 | 4.121 | 16.745 | 1.00 | 25.95 |
| ATOM | 80 | CA | LEU | 1473 | -11.961 | 3.740 | 18.129 | 1.00 | 27.45 |
| ATOM | 81 | CB | LEU | 1473 | -10.707 | 3.311 | 18.890 | 1.00 | 24.99 |
| ATOM | 82 | CG | LEU | 1473 | -10.958 | 3.090 | 20.392 | 1.00 | 21.80 |
| ATOM | 83 | CD1 | LEU | 1473 | -11.551 | 1.696 | 20.627 | 1.00 | 20.63 |
| ATOM | 84 | CD2 | LEU | 1473 | -9.646 | 3.199 | 21.157 | 1.00 | 22.34 |
| ATOM | 85 | C | LEU | 1473 | -12.478 | 5.008 | 18.752 | 1.00 | 29.33 |
| ATOM | 86 | O | LEU | 1473 | -12.007 | 6.101 | 18.405 | 1.00 | 27.56 |
| ATOM | 87 | N | PRO | 1474 | -13.529 | 4.896 | 19.585 | 1.00 | 30.07 |
| ATOM | 88 | CD | PRO | 1474 | -14.380 | 3.704 | 19.737 | 1.00 | 29.18 |
| ATOM | 89 | CA | PRO | 1474 | -14.124 | 6.051 | 20.267 | 1.00 | 29.03 |
| ATOM | 90 | CB | PRO | 1474 | -15.266 | 5.406 | 21.062 | 1.00 | 26.83 |
| ATOM | 91 | CG | PRO | 1474 | -15.701 | 4.307 | 20.158 | 1.00 | 26.35 |
| ATOM | 92 | C | PRO | 1474 | -13.099 | 6.715 | 21.178 | 1.00 | 31.01 |
| ATOM | 93 | O | PRO | 1474 | -12.310 | 6.042 | 21.850 | 1.00 | 33.14 |
| ATOM | 94 | N | ARG | 1475 | -13.110 | 8.038 | 21.178 | 1.00 | 31.33 |
| ATOM | 95 | CA | ARG | 1475 | -12.181 | 8.810 | 21.973 | 1.00 | 32.99 |
| ATOM | 96 | CB | ARG | 1475 | -12.442 | 10.292 | 21.791 | 1.00 | 35.87 |
| ATOM | 97 | CG | ARG | 1475 | -12.082 | 10.729 | 20.413 | 1.00 | 43.88 |
| ATOM | 98 | CD | ARG | 1475 | -11.984 | 12.228 | 20.247 | 1.00 | 44.84 |

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ATOM     99  NE  ARG  1475     -11.665  12.499  18.846  1.00 48.59
ATOM    100  CZ  ARG  1475     -10.435  12.663  18.374  1.00 46.00
ATOM    101  NH1 ARG  1475      -9.400  12.618  19.202  1.00 46.56
ATOM    102  NH2 ARG  1475     -10.241  12.746  17.065  1.00 44.18
ATOM    103  C   ARG  1475     -12.175   8.456  23.442  1.00 35.47
ATOM    104  O   ARG  1475     -11.115   8.400  24.072  1.00 37.44
ATOM    105  N   ASP  1476     -13.347   8.134  23.974  1.00 35.04
ATOM    106  CA  ASP  1476     -13.468   7.800  25.380  1.00 34.30
ATOM    107  CB  ASP  1476     -14.940   7.853  25.797  1.00 36.89
ATOM    108  CG  ASP  1476     -15.796   6.818  25.089  1.00 38.67
ATOM    109  OD1 ASP  1476     -15.288   6.056  24.234  1.00 41.19
ATOM    110  OD2 ASP  1476     -16.995   6.758  25.406  1.00 48.08
ATOM    111  C   ASP  1476     -12.858   6.457  25.770  1.00 33.67
ATOM    112  O   ASP  1476     -12.830   6.109  26.949  1.00 36.57
ATOM    113  N   ARG  1477     -12.441   5.670  24.781  1.00 32.72
ATOM    114  CA  ARG  1477     -11.828   4.370  25.033  1.00 29.68
ATOM    115  CB  ARG  1477     -12.117   3.418  23.886  1.00 25.53
ATOM    116  CG  ARG  1477     -13.564   3.189  23.599  1.00 23.83
ATOM    117  CD  ARG  1477     -14.234   2.525  24.772  1.00 26.80
ATOM    118  NE  ARG  1477     -14.493   3.485  25.842  1.00 27.24
ATOM    119  CZ  ARG  1477     -14.818   3.145  27.085  1.00 27.41
ATOM    120  NH1 ARG  1477     -14.931   1.874  27.438  1.00 29.00
ATOM    121  NH2 ARG  1477     -15.005   4.095  27.985  1.00 25.85
ATOM    122  C   ARG  1477     -10.316   4.489  25.177  1.00 30.44
ATOM    123  O   ARG  1477      -9.616   3.515  25.461  1.00 32.78
ATOM    124  N   LEU  1478      -9.800   5.690  25.002  1.00 30.39
ATOM    125  CA  LEU  1478      -8.370   5.883  25.080  1.00 31.96
ATOM    126  CB  LEU  1478      -7.886   6.508  23.771  1.00 30.43
ATOM    127  CG  LEU  1478      -6.400   6.424  23.431  1.00 31.90
ATOM    128  CD1 LEU  1478      -5.939   4.964  23.382  1.00 28.92
ATOM    129  CD2 LEU  1478      -6.159   7.115  22.102  1.00 33.55
ATOM    130  C   LEU  1478      -7.974   6.757  26.265  1.00 33.60
ATOM    131  O   LEU  1478      -8.193   7.972  26.251  1.00 33.96
ATOM    132  N   VAL  1479      -7.416   6.140  27.305  1.00 33.54
ATOM    133  CA  VAL  1479      -6.974   6.902  28.468  1.00 32.52
ATOM    134  CB  VAL  1479      -7.085   6.089  29.757  1.00 32.76
ATOM    135  CG1 VAL  1479      -6.728   6.973  30.926  1.00 33.27
ATOM    136  CG2 VAL  1479      -8.493   5.537  29.913  1.00 30.15
ATOM    137  C   VAL  1479      -5.529   7.341  28.239  1.00 34.24
ATOM    138  O   VAL  1479      -4.581   6.546  28.350  1.00 32.24
ATOM    139  N   LEU  1480      -5.381   8.607  27.867  1.00 35.88
ATOM    140  CA  LEU  1480      -4.077   9.192  27.569  1.00 38.43
ATOM    141  CB  LEU  1480      -4.241  10.541  26.855  1.00 36.93
ATOM    142  CG  LEU  1480      -4.828  10.535  25.435  1.00 35.67
ATOM    143  CD1 LEU  1480      -4.762  11.952  24.907  1.00 32.47
ATOM    144  CD2 LEU  1480      -4.037   9.613  24.499  1.00 33.60
ATOM    145  C   LEU  1480      -3.144   9.324  28.768  1.00 39.70
ATOM    146  O   LEU  1480      -3.511   9.912  29.784  1.00 39.88
ATOM    147  N   GLY  1481      -1.912   8.842  28.610  1.00 39.70
ATOM    148  CA  GLY  1481      -0.960   8.896  29.700  1.00 41.31
ATOM    149  C   GLY  1481       0.349   9.633  29.474  1.00 44.39
ATOM    150  O   GLY  1481       0.429  10.626  28.744  1.00 45.69
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 151 | N | LYS | 1482 | 1.389 | 9.122 | 30.124 | 1.00 | 44.73 |
| ATOM | 152 | CA | LYS | 1482 | 2.728 | 9.700 | 30.069 | 1.00 | 46.91 |
| ATOM | 153 | CB | LYS | 1482 | 3.649 | 8.934 | 31.023 | 1.00 | 51.20 |
| ATOM | 154 | CG | LYS | 1482 | 5.135 | 9.056 | 30.744 | 1.00 | 57.10 |
| ATOM | 155 | CD | LYS | 1482 | 5.878 | 7.826 | 31.248 | 1.00 | 60.81 |
| ATOM | 156 | CE | LYS | 1482 | 5.430 | 6.567 | 30.515 | 1.00 | 61.24 |
| ATOM | 157 | NZ | LYS | 1482 | 6.235 | 5.375 | 30.912 | 1.00 | 65.39 |
| ATOM | 158 | C | LYS | 1482 | 3.370 | 9.782 | 28.681 | 1.00 | 46.09 |
| ATOM | 159 | O | LYS | 1482 | 3.440 | 8.782 | 27.944 | 1.00 | 42.98 |
| ATOM | 160 | N | PRO | 1483 | 3.886 | 10.969 | 28.324 | 1.00 | 46.65 |
| ATOM | 161 | CD | PRO | 1483 | 3.910 | 12.184 | 29.152 | 1.00 | 46.11 |
| ATOM | 162 | CA | PRO | 1483 | 4.536 | 11.212 | 27.036 | 1.00 | 45.96 |
| ATOM | 163 | CB | PRO | 1483 | 5.015 | 12.660 | 27.172 | 1.00 | 43.59 |
| ATOM | 164 | CG | PRO | 1483 | 4.041 | 13.253 | 28.122 | 1.00 | 45.37 |
| ATOM | 165 | C | PRO | 1483 | 5.739 | 10.279 | 26.912 | 1.00 | 46.43 |
| ATOM | 166 | O | PRO | 1483 | 6.506 | 10.139 | 27.861 | 1.00 | 44.77 |
| ATOM | 167 | N | LEU | 1484 | 5.844 | 9.579 | 25.786 | 1.00 | 48.21 |
| ATOM | 168 | CA | LEU | 1484 | 6.978 | 8.684 | 25.554 | 1.00 | 50.46 |
| ATOM | 169 | CB | LEU | 1484 | 6.543 | 7.426 | 24.811 | 1.00 | 49.38 |
| ATOM | 170 | CG | LEU | 1484 | 5.655 | 6.437 | 25.576 | 1.00 | 50.15 |
| ATOM | 171 | CD1 | LEU | 1484 | 5.067 | 5.422 | 24.615 | 1.00 | 44.90 |
| ATOM | 172 | CD2 | LEU | 1484 | 6.446 | 5.750 | 26.669 | 1.00 | 44.60 |
| ATOM | 173 | C | LEU | 1484 | 8.058 | 9.419 | 24.764 | 1.00 | 53.33 |
| ATOM | 174 | O | LEU | 1484 | 9.241 | 9.116 | 24.896 | 1.00 | 51.94 |
| ATOM | 175 | N | GLY | 1485 | 7.643 | 10.376 | 23.931 | 1.00 | 57.68 |
| ATOM | 176 | CA | GLY | 1485 | 8.603 | 11.140 | 23.148 | 1.00 | 60.27 |
| ATOM | 177 | C | GLY | 1485 | 7.997 | 11.946 | 22.016 | 1.00 | 62.66 |
| ATOM | 178 | O | GLY | 1485 | 6.774 | 12.090 | 21.924 | 1.00 | 64.91 |
| ATOM | 179 | N | GLN | 1491 | 4.704 | 14.425 | 18.904 | 1.00 | 47.86 |
| ATOM | 180 | CA | GLN | 1491 | 4.339 | 13.868 | 20.206 | 1.00 | 44.42 |
| ATOM | 181 | CB | GLN | 1491 | 3.373 | 14.829 | 20.918 | 1.00 | 44.31 |
| ATOM | 182 | C | GLN | 1491 | 3.755 | 12.433 | 20.170 | 1.00 | 43.09 |
| ATOM | 183 | O | GLN | 1491 | 2.807 | 12.150 | 19.426 | 1.00 | 43.67 |
| ATOM | 184 | N | VAL | 1492 | 4.338 | 11.542 | 20.974 | 1.00 | 40.40 |
| ATOM | 185 | CA | VAL | 1492 | 3.903 | 10.143 | 21.101 | 1.00 | 39.95 |
| ATOM | 186 | CB | VAL | 1492 | 4.962 | 9.119 | 20.673 | 1.00 | 37.64 |
| ATOM | 187 | CG1 | VAL | 1492 | 4.416 | 7.721 | 20.897 | 1.00 | 34.94 |
| ATOM | 188 | CG2 | VAL | 1492 | 5.336 | 9.296 | 19.233 | 1.00 | 40.26 |
| ATOM | 189 | C | VAL | 1492 | 3.720 | 9.905 | 22.586 | 1.00 | 40.23 |
| ATOM | 190 | O | VAL | 1492 | 4.679 | 10.038 | 23.355 | 1.00 | 40.41 |
| ATOM | 191 | N | VAL | 1493 | 2.516 | 9.518 | 22.993 | 1.00 | 38.15 |
| ATOM | 192 | CA | VAL | 1493 | 2.250 | 9.291 | 24.405 | 1.00 | 37.11 |
| ATOM | 193 | CB | VAL | 1493 | 1.131 | 10.245 | 24.924 | 1.00 | 37.83 |
| ATOM | 194 | CG1 | VAL | 1493 | 1.386 | 11.656 | 24.422 | 1.00 | 36.45 |
| ATOM | 195 | CG2 | VAL | 1493 | -0.252 | 9.769 | 24.508 | 1.00 | 39.28 |
| ATOM | 196 | C | VAL | 1493 | 1.854 | 7.844 | 24.701 | 1.00 | 36.02 |
| ATOM | 197 | O | VAL | 1493 | 1.450 | 7.118 | 23.797 | 1.00 | 37.17 |
| ATOM | 198 | N | LEU | 1494 | 2.052 | 7.418 | 25.944 | 1.00 | 32.77 |
| ATOM | 199 | CA | LEU | 1494 | 1.645 | 6.081 | 26.335 | 1.00 | 30.87 |
| ATOM | 200 | CB | LEU | 1494 | 2.445 | 5.587 | 27.550 | 1.00 | 27.22 |
| ATOM | 201 | CG | LEU | 1494 | 1.970 | 4.250 | 28.141 | 1.00 | 28.67 |
| ATOM | 202 | CD1 | LEU | 1494 | 2.124 | 3.132 | 27.129 | 1.00 | 27.40 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 203 | CD2 | LEU | 1494 | 2.736 | 3.904 | 29.377 | 1.00 | 28.84 |
| ATOM | 204 | C | LEU | 1494 | 0.173 | 6.256 | 26.701 | 1.00 | 31.18 |
| ATOM | 205 | O | LEU | 1494 | -0.249 | 7.344 | 27.119 | 1.00 | 30.88 |
| ATOM | 206 | N | ALA | 1495 | -0.626 | 5.223 | 26.477 | 1.00 | 30.40 |
| ATOM | 207 | CA | ALA | 1495 | -2.044 | 5.307 | 26.817 | 1.00 | 28.30 |
| ATOM | 208 | CB | ALA | 1495 | -2.815 | 5.999 | 25.691 | 1.00 | 27.35 |
| ATOM | 209 | C | ALA | 1495 | -2.608 | 3.919 | 27.057 | 1.00 | 26.32 |
| ATOM | 210 | O | ALA | 1495 | -1.926 | 2.915 | 26.846 | 1.00 | 24.54 |
| ATOM | 211 | N | GLU | 1496 | -3.836 | 3.867 | 27.552 | 1.00 | 28.11 |
| ATOM | 212 | CA | GLU | 1496 | -4.514 | 2.603 | 27.793 | 1.00 | 29.22 |
| ATOM | 213 | CB | GLU | 1496 | -4.841 | 2.441 | 29.272 | 1.00 | 31.77 |
| ATOM | 214 | CG | GLU | 1496 | -3.627 | 2.233 | 30.140 | 1.00 | 37.26 |
| ATOM | 215 | CD | GLU | 1496 | -3.950 | 2.405 | 31.613 | 1.00 | 39.77 |
| ATOM | 216 | OE1 | GLU | 1496 | -4.322 | 3.534 | 31.999 | 1.00 | 37.54 |
| ATOM | 217 | OE2 | GLU | 1496 | -3.835 | 1.417 | 32.378 | 1.00 | 41.52 |
| ATOM | 218 | C | GLU | 1496 | -5.799 | 2.594 | 26.970 | 1.00 | 29.76 |
| ATOM | 219 | O | GLU | 1496 | -6.593 | 3.543 | 27.020 | 1.00 | 31.39 |
| ATOM | 220 | N | ALA | 1497 | -5.961 | 1.561 | 26.153 | 1.00 | 29.55 |
| ATOM | 221 | CA | ALA | 1497 | -7.139 | 1.426 | 25.324 | 1.00 | 28.69 |
| ATOM | 222 | CB | ALA | 1497 | -6.742 | 0.969 | 23.930 | 1.00 | 23.86 |
| ATOM | 223 | C | ALA | 1497 | -8.068 | 0.418 | 25.965 | 1.00 | 29.51 |
| ATOM | 224 | O | ALA | 1497 | -7.657 | -0.702 | 26.278 | 1.00 | 30.40 |
| ATOM | 225 | N | ILE | 1498 | -9.313 | 0.823 | 26.201 | 1.00 | 31.33 |
| ATOM | 226 | CA | ILE | 1498 | -10.302 | -0.064 | 26.811 | 1.00 | 32.30 |
| ATOM | 227 | CB | ILE | 1498 | -11.359 | 0.727 | 27.619 | 1.00 | 33.61 |
| ATOM | 228 | CG2 | ILE | 1498 | -12.233 | -0.246 | 28.439 | 1.00 | 34.55 |
| ATOM | 229 | CG1 | ILE | 1498 | -10.690 | 1.745 | 28.545 | 1.00 | 31.99 |
| ATOM | 230 | CD1 | ILE | 1498 | -11.663 | 2.730 | 29.155 | 1.00 | 26.68 |
| ATOM | 231 | C | ILE | 1498 | -11.023 | -0.777 | 25.673 | 1.00 | 32.69 |
| ATOM | 232 | O | ILE | 1498 | -11.644 | -0.134 | 24.838 | 1.00 | 32.03 |
| ATOM | 233 | N | GLY | 1499 | -10.917 | -2.095 | 25.610 | 1.00 | 37.34 |
| ATOM | 234 | CA | GLY | 1499 | -11.588 | -2.822 | 24.554 | 1.00 | 44.45 |
| ATOM | 235 | C | GLY | 1499 | -10.709 | -3.193 | 23.372 | 1.00 | 50.75 |
| ATOM | 236 | O | GLY | 1499 | -9.993 | -4.205 | 23.438 | 1.00 | 53.68 |
| ATOM | 237 | N | LEU | 1500 | -10.729 | -2.370 | 22.321 | 1.00 | 51.14 |
| ATOM | 238 | CA | LEU | 1500 | -9.963 | -2.613 | 21.087 | 1.00 | 51.15 |
| ATOM | 239 | CB | LEU | 1500 | -8.445 | -2.677 | 21.345 | 1.00 | 50.85 |
| ATOM | 240 | CG | LEU | 1500 | -7.516 | -1.463 | 21.166 | 1.00 | 49.05 |
| ATOM | 241 | CD1 | LEU | 1500 | -6.082 | -1.946 | 21.263 | 1.00 | 44.92 |
| ATOM | 242 | CD2 | LEU | 1500 | -7.703 | -0.783 | 19.824 | 1.00 | 44.03 |
| ATOM | 243 | C | LEU | 1500 | -10.420 | -3.891 | 20.376 | 1.00 | 50.50 |
| ATOM | 244 | O | LEU | 1500 | -10.544 | -4.966 | 20.984 | 1.00 | 49.92 |
| ATOM | 245 | N | PRO | 1505 | -13.321 | -5.777 | 25.373 | 1.00 | 48.57 |
| ATOM | 246 | CD | PRO | 1505 | -13.937 | -7.111 | 25.286 | 1.00 | 50.09 |
| ATOM | 247 | CA | PRO | 1505 | -14.289 | -4.776 | 25.848 | 1.00 | 46.31 |
| ATOM | 248 | CB | PRO | 1505 | -15.630 | -5.503 | 25.710 | 1.00 | 45.25 |
| ATOM | 249 | CG | PRO | 1505 | -15.271 | -6.918 | 26.025 | 1.00 | 48.85 |
| ATOM | 250 | C | PRO | 1505 | -14.010 | -4.321 | 27.294 | 1.00 | 43.31 |
| ATOM | 251 | O | PRO | 1505 | -14.001 | -3.122 | 27.571 | 1.00 | 42.84 |
| ATOM | 252 | N | ASN | 1506 | -13.712 | -5.272 | 28.178 | 1.00 | 40.46 |
| ATOM | 253 | CA | ASN | 1506 | -13.430 | -4.945 | 29.571 | 1.00 | 42.33 |
| ATOM | 254 | CB | ASN | 1506 | -14.302 | -5.776 | 30.512 | 1.00 | 43.55 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 255 | CG | ASN | 1506 | -15.760 | -5.436 | 30.382 | 1.00 | 42.68 |
| ATOM | 256 | OD1 | ASN | 1506 | -16.141 | -4.269 | 30.316 | 1.00 | 47.11 |
| ATOM | 257 | ND2 | ASN | 1506 | -16.591 | -6.461 | 30.323 | 1.00 | 45.66 |
| ATOM | 258 | C | ASN | 1506 | -11.962 | -5.097 | 29.957 | 1.00 | 42.89 |
| ATOM | 259 | O | ASN | 1506 | -11.617 | -5.221 | 31.137 | 1.00 | 43.23 |
| ATOM | 260 | N | ARG | 1507 | -11.099 | -5.066 | 28.949 | 1.00 | 42.72 |
| ATOM | 261 | CA | ARG | 1507 | -9.661 | -5.186 | 29.145 | 1.00 | 42.24 |
| ATOM | 262 | CB | ARG | 1507 | -9.144 | -6.384 | 28.353 | 1.00 | 50.39 |
| ATOM | 263 | CG | ARG | 1507 | -9.407 | -7.728 | 28.992 | 1.00 | 60.88 |
| ATOM | 264 | CD | ARG | 1507 | -8.357 | -8.063 | 30.038 | 1.00 | 67.47 |
| ATOM | 265 | NE | ARG | 1507 | -8.566 | -9.401 | 30.574 | 1.00 | 74.19 |
| ATOM | 266 | CZ | ARG | 1507 | -8.012 | -9.861 | 31.691 | 1.00 | 79.97 |
| ATOM | 267 | NH1 | ARG | 1507 | -7.193 | -9.093 | 32.406 | 1.00 | 81.67 |
| ATOM | 268 | NH2 | ARG | 1507 | -8.338 | -11.068 | 32.134 | 1.00 | 82.38 |
| ATOM | 269 | C | ARG | 1507 | -8.982 | -3.940 | 28.611 | 1.00 | 38.15 |
| ATOM | 270 | O | ARG | 1507 | -9.458 | -3.354 | 27.642 | 1.00 | 36.46 |
| ATOM | 271 | N | VAL | 1508 | -7.927 | -3.491 | 29.279 | 1.00 | 35.19 |
| ATOM | 272 | CA | VAL | 1508 | -7.190 | -2.335 | 28.782 | 1.00 | 33.82 |
| ATOM | 273 | CB | VAL | 1508 | -6.824 | -1.296 | 29.883 | 1.00 | 30.19 |
| ATOM | 274 | CG1 | VAL | 1508 | -8.072 | -0.723 | 30.498 | 1.00 | 34.68 |
| ATOM | 275 | CG2 | VAL | 1508 | -5.948 | -1.900 | 30.938 | 1.00 | 28.53 |
| ATOM | 276 | C | VAL | 1508 | -5.912 | -2.869 | 28.155 | 1.00 | 33.91 |
| ATOM | 277 | O | VAL | 1508 | -5.392 | -3.926 | 28.555 | 1.00 | 34.02 |
| ATOM | 278 | N | THR | 1509 | -5.427 | -2.152 | 27.154 | 1.00 | 31.32 |
| ATOM | 279 | CA | THR | 1509 | -4.206 | -2.527 | 26.476 | 1.00 | 30.47 |
| ATOM | 280 | CB | THR | 1509 | -4.492 | -3.015 | 25.031 | 1.00 | 30.88 |
| ATOM | 281 | OG1 | THR | 1509 | -5.522 | -4.008 | 25.066 | 1.00 | 33.90 |
| ATOM | 282 | CG2 | THR | 1509 | -3.255 | -3.648 | 24.411 | 1.00 | 24.49 |
| ATOM | 283 | C | THR | 1509 | -3.323 | -1.300 | 26.419 | 1.00 | 28.74 |
| ATOM | 284 | O | THR | 1509 | -3.774 | -0.219 | 26.039 | 1.00 | 27.29 |
| ATOM | 285 | N | LYS | 1510 | -2.092 | -1.432 | 26.893 | 1.00 | 29.17 |
| ATOM | 286 | CA | LYS | 1510 | -1.162 | -0.325 | 26.831 | 1.00 | 30.55 |
| ATOM | 287 | CB | LYS | 1510 | 0.092 | -0.595 | 27.648 | 1.00 | 27.23 |
| ATOM | 288 | CG | LYS | 1510 | -0.117 | -0.460 | 29.135 | 1.00 | 34.33 |
| ATOM | 289 | CD | LYS | 1510 | 1.191 | -0.614 | 29.896 | 1.00 | 40.49 |
| ATOM | 290 | CE | LYS | 1510 | 1.065 | -1.603 | 31.062 | 1.00 | 48.28 |
| ATOM | 291 | NZ | LYS | 1510 | 0.318 | -1.067 | 32.245 | 1.00 | 51.03 |
| ATOM | 292 | C | LYS | 1510 | -0.813 | -0.213 | 25.355 | 1.00 | 29.64 |
| ATOM | 293 | O | LYS | 1510 | -0.521 | -1.218 | 24.700 | 1.00 | 28.00 |
| ATOM | 294 | N | VAL | 1511 | -0.904 | 1.004 | 24.836 | 1.00 | 30.10 |
| ATOM | 295 | CA | VAL | 1511 | -0.625 | 1.305 | 23.446 | 1.00 | 30.13 |
| ATOM | 296 | CB | VAL | 1511 | -1.951 | 1.464 | 22.636 | 1.00 | 31.39 |
| ATOM | 297 | CG1 | VAL | 1511 | -2.719 | 0.143 | 22.615 | 1.00 | 30.42 |
| ATOM | 298 | CG2 | VAL | 1511 | -2.829 | 2.629 | 23.223 | 1.00 | 28.08 |
| ATOM | 299 | C | VAL | 1511 | 0.150 | 2.626 | 23.365 | 1.00 | 30.51 |
| ATOM | 300 | O | VAL | 1511 | 0.274 | 3.346 | 24.360 | 1.00 | 31.09 |
| ATOM | 301 | N | ALA | 1512 | 0.679 | 2.935 | 22.185 | 1.00 | 28.30 |
| ATOM | 302 | CA | ALA | 1512 | 1.408 | 4.173 | 21.979 | 1.00 | 25.23 |
| ATOM | 303 | CB | ALA | 1512 | 2.740 | 3.889 | 21.331 | 1.00 | 23.82 |
| ATOM | 304 | C | ALA | 1512 | 0.535 | 5.012 | 21.057 | 1.00 | 25.50 |
| ATOM | 305 | O | ALA | 1512 | 0.033 | 4.515 | 20.061 | 1.00 | 27.06 |
| ATOM | 306 | N | VAL | 1513 | 0.351 | 6.281 | 21.404 | 1.00 | 29.37 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 307 | CA | VAL | 1513 | -0.477 | 7.199 | 20.625 | 1.00 | 31.53 |
| ATOM | 308 | CB | VAL | 1513 | -1.588 | 7.843 | 21.504 | 1.00 | 32.26 |
| ATOM | 309 | CG1 | VAL | 1513 | -2.453 | 8.775 | 20.684 | 1.00 | 34.37 |
| ATOM | 310 | CG2 | VAL | 1513 | -2.452 | 6.776 | 22.152 | 1.00 | 33.42 |
| ATOM | 311 | C | VAL | 1513 | 0.347 | 8.328 | 20.006 | 1.00 | 33.34 |
| ATOM | 312 | O | VAL | 1513 | 1.030 | 9.064 | 20.719 | 1.00 | 32.35 |
| ATOM | 313 | N | LYS | 1514 | 0.321 | 8.423 | 18.680 | 1.00 | 36.65 |
| ATOM | 314 | CA | LYS | 1514 | 1.022 | 9.466 | 17.929 | 1.00 | 37.26 |
| ATOM | 315 | CB | LYS | 1514 | 1.541 | 8.917 | 16.606 | 1.00 | 36.21 |
| ATOM | 316 | CG | LYS | 1514 | 2.524 | 7.792 | 16.800 | 1.00 | 39.32 |
| ATOM | 317 | CD | LYS | 1514 | 2.725 | 6.998 | 15.535 | 1.00 | 42.59 |
| ATOM | 318 | CE | LYS | 1514 | 3.245 | 7.860 | 14.416 | 1.00 | 44.71 |
| ATOM | 319 | NZ | LYS | 1514 | 4.408 | 8.680 | 14.844 | 1.00 | 38.78 |
| ATOM | 320 | C | LYS | 1514 | 0.020 | 10.574 | 17.653 | 1.00 | 37.21 |
| ATOM | 321 | O | LYS | 1514 | -1.095 | 10.305 | 17.192 | 1.00 | 37.39 |
| ATOM | 322 | N | MET | 1515 | 0.433 | 11.812 | 17.908 | 1.00 | 39.05 |
| ATOM | 323 | CA | MET | 1515 | -0.419 | 12.981 | 17.713 | 1.00 | 41.68 |
| ATOM | 324 | CB | MET | 1515 | -1.162 | 13.299 | 18.991 | 1.00 | 41.07 |
| ATOM | 325 | CG | MET | 1515 | -0.251 | 13.641 | 20.139 | 1.00 | 40.69 |
| ATOM | 326 | SD | MET | 1515 | -1.271 | 13.763 | 21.571 | 1.00 | 41.18 |
| ATOM | 327 | CE | MET | 1515 | -1.523 | 12.018 | 21.959 | 1.00 | 40.98 |
| ATOM | 328 | C | MET | 1515 | 0.397 | 14.197 | 17.321 | 1.00 | 44.66 |
| ATOM | 329 | O | MET | 1515 | 1.606 | 14.255 | 17.550 | 1.00 | 43.83 |
| ATOM | 330 | N | LEU | 1516 | -0.288 | 15.182 | 16.747 | 1.00 | 50.63 |
| ATOM | 331 | CA | LEU | 1516 | 0.349 | 16.423 | 16.312 | 1.00 | 52.21 |
| ATOM | 332 | CB | LEU | 1516 | -0.513 | 17.129 | 15.255 | 1.00 | 50.18 |
| ATOM | 333 | CG | LEU | 1516 | -0.757 | 16.463 | 13.904 | 1.00 | 50.25 |
| ATOM | 334 | CD1 | LEU | 1516 | -1.733 | 17.298 | 13.114 | 1.00 | 51.02 |
| ATOM | 335 | CD2 | LEU | 1516 | 0.555 | 16.329 | 13.163 | 1.00 | 51.60 |
| ATOM | 336 | C | LEU | 1516 | 0.549 | 17.391 | 17.473 | 1.00 | 54.25 |
| ATOM | 337 | O | LEU | 1516 | -0.143 | 17.326 | 18.488 | 1.00 | 52.52 |
| ATOM | 338 | N | LYS | 1517 | 1.500 | 18.299 | 17.302 | 1.00 | 59.09 |
| ATOM | 339 | CA | LYS | 1517 | 1.773 | 19.315 | 18.313 | 1.00 | 62.57 |
| ATOM | 340 | CB | LYS | 1517 | 3.220 | 19.813 | 18.222 | 1.00 | 66.29 |
| ATOM | 341 | CG | LYS | 1517 | 4.281 | 18.810 | 18.663 | 1.00 | 70.96 |
| ATOM | 342 | CD | LYS | 1517 | 5.666 | 19.197 | 18.130 | 1.00 | 74.61 |
| ATOM | 343 | CE | LYS | 1517 | 6.711 | 18.118 | 18.414 | 1.00 | 78.21 |
| ATOM | 344 | NZ | LYS | 1517 | 8.020 | 18.410 | 17.751 | 1.00 | 77.95 |
| ATOM | 345 | C | LYS | 1517 | 0.824 | 20.474 | 18.037 | 1.00 | 63.07 |
| ATOM | 346 | O | LYS | 1517 | 0.226 | 20.557 | 16.960 | 1.00 | 63.68 |
| ATOM | 347 | N | SER | 1518 | 0.720 | 21.391 | 18.987 | 1.00 | 64.54 |
| ATOM | 348 | CA | SER | 1518 | -0.167 | 22.543 | 18.848 | 1.00 | 67.29 |
| ATOM | 349 | CB | SER | 1518 | -0.085 | 23.439 | 20.090 | 1.00 | 65.14 |
| ATOM | 350 | C | SER | 1518 | 0.124 | 23.382 | 17.609 | 1.00 | 69.48 |
| ATOM | 351 | O | SER | 1518 | -0.798 | 23.843 | 16.938 | 1.00 | 71.85 |
| ATOM | 352 | N | ASP | 1519 | 1.402 | 23.530 | 17.280 | 1.00 | 70.88 |
| ATOM | 353 | CA | ASP | 1519 | 1.802 | 24.326 | 16.127 | 1.00 | 72.00 |
| ATOM | 354 | CB | ASP | 1519 | 3.162 | 24.973 | 16.385 | 1.00 | 72.61 |
| ATOM | 355 | C | ASP | 1519 | 1.861 | 23.548 | 14.817 | 1.00 | 72.32 |
| ATOM | 356 | O | ASP | 1519 | 2.432 | 24.035 | 13.844 | 1.00 | 73.72 |
| ATOM | 357 | N | ALA | 1520 | 1.322 | 22.332 | 14.798 | 1.00 | 72.11 |
| ATOM | 358 | CA | ALA | 1520 | 1.344 | 21.508 | 13.595 | 1.00 | 71.13 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 359 | CB | ALA | 1520 | 0.659 | 20.173 | 13.855 | 1.00 | 71.01 |
| ATOM | 360 | C | ALA | 1520 | 0.666 | 22.242 | 12.440 | 1.00 | 69.96 |
| ATOM | 361 | O | ALA | 1520 | -0.314 | 22.962 | 12.639 | 1.00 | 71.41 |
| ATOM | 362 | N | THR | 1521 | 1.230 | 22.101 | 11.249 | 1.00 | 67.39 |
| ATOM | 363 | CA | THR | 1521 | 0.676 | 22.726 | 10.064 | 1.00 | 66.23 |
| ATOM | 364 | CB | THR | 1521 | 1.798 | 23.167 | 9.132 | 1.00 | 66.40 |
| ATOM | 365 | OG1 | THR | 1521 | 2.521 | 22.016 | 8.680 | 1.00 | 70.07 |
| ATOM | 366 | CG2 | THR | 1521 | 2.741 | 24.070 | 9.867 | 1.00 | 66.67 |
| ATOM | 367 | C | THR | 1521 | -0.150 | 21.665 | 9.364 | 1.00 | 65.62 |
| ATOM | 368 | O | THR | 1521 | -0.093 | 20.493 | 9.740 | 1.00 | 66.78 |
| ATOM | 369 | N | GLU | 1522 | -0.893 | 22.057 | 8.330 | 1.00 | 63.60 |
| ATOM | 370 | CA | GLU | 1522 | -1.698 | 21.095 | 7.584 | 1.00 | 62.25 |
| ATOM | 371 | CB | GLU | 1522 | -2.560 | 21.802 | 6.531 | 1.00 | 64.02 |
| ATOM | 372 | C | GLU | 1522 | -0.768 | 20.051 | 6.942 | 1.00 | 60.41 |
| ATOM | 373 | O | GLU | 1522 | -1.161 | 18.906 | 6.738 | 1.00 | 61.94 |
| ATOM | 374 | N | LYS | 1523 | 0.475 | 20.441 | 6.662 | 1.00 | 56.47 |
| ATOM | 375 | CA | LYS | 1523 | 1.449 | 19.529 | 6.080 | 1.00 | 54.53 |
| ATOM | 376 | CB | LYS | 1523 | 2.739 | 20.273 | 5.713 | 1.00 | 57.44 |
| ATOM | 377 | CG | LYS | 1523 | 3.897 | 19.381 | 5 219 | 1.00 | 61.49 |
| ATOM | 378 | CD | LYS | 1523 | 3.482 | 18.451 | 4.071 | 1.00 | 64.66 |
| ATOM | 379 | CE | LYS | 1523 | 4.681 | 17.723 | 3.469 | 1.00 | 68.18 |
| ATOM | 380 | NZ | LYS | 1523 | 4.252 | 16.704 | 2.458 | 1.00 | 73.23 |
| ATOM | 381 | C | LYS | 1523 | 1.728 | 18.474 | 7.135 | 1.00 | 52.30 |
| ATOM | 382 | O | LYS | 1523 | 1.757 | 17.280 | 6.832 | 1.00 | 54.59 |
| ATOM | 383 | N | ASP | 1524 | 1.899 | 18.921 | 8.376 | 1.00 | 47.78 |
| ATOM | 384 | CA | ASP | 1524 | 2.147 | 18.023 | 9.493 | 1.00 | 45.55 |
| ATOM | 385 | CB | ASP | 1524 | 2.380 | 18.815 | 10.783 | 1.00 | 47.64 |
| ATOM | 386 | CG | ASP | 1524 | 3.744 | 19.511 | 10.817 | 1.00 | 49.50 |
| ATOM | 387 | OD1 | ASP | 1524 | 3.849 | 20.580 | 11.460 | 1.00 | 47.22 |
| ATOM | 388 | OD2 | ASP | 1524 | 4.715 | 18.984 | 10.230 | 1.00 | 52.84 |
| ATOM | 389 | C | ASP | 1524 | 0.968 | 17.054 | 9.661 | 1.00 | 43.55 |
| ATOM | 390 | O | ASP | 1524 | 1.157 | 15.890 | 10.007 | 1.00 | 43.98 |
| ATOM | 391 | N | LEU | 1525 | -0.240 | 17.541 | 9.391 | 1.00 | 40.77 |
| ATOM | 392 | CA | LEU | 1525 | -1.438 | 16.713 | 9.483 | 1.00 | 40.28 |
| ATOM | 393 | CB | LEU | 1525 | -2.701 | 17.592 | 9.411 | 1.00 | 40.54 |
| ATOM | 394 | CG | LEU | 1525 | -4.100 | 16.957 | 9.403 | 1.00 | 40.33 |
| ATOM | 395 | CD1 | LEU | 1525 | -4.289 | 15.933 | 10.514 | 1.00 | 42.75 |
| ATOM | 396 | CD2 | LEU | 1525 | -5.120 | 18.044 | 9.524 | 1.00 | 36.98 |
| ATOM | 397 | C | LEU | 1525 | -1.417 | 15.699 | 8.343 | 1.00 | 40.19 |
| ATOM | 398 | O | LEU | 1525 | -1.682 | 14.525 | 8.557 | 1.00 | 41.90 |
| ATOM | 399 | N | SER | 1526 | -1.064 | 16.158 | 7.147 | 1.00 | 42.13 |
| ATOM | 400 | CA | SER | 1526 | -1.002 | 15.315 | 5.954 | 1.00 | 44.75 |
| ATOM | 401 | CB | SER | 1526 | -0.582 | 16.136 | 4.723 | 1.00 | 49.61 |
| ATOM | 402 | OG | SER | 1526 | -1.538 | 17.100 | 4.352 | 1.00 | 59.95 |
| ATOM | 403 | C | SER | 1526 | -0.007 | 14.193 | 6.144 | 1.00 | 42.71 |
| ATOM | 404 | O | SER | 1526 | -0.297 | 13.047 | 5.840 | 1.00 | 45.33 |
| ATOM | 405 | N | ASP | 1527 | 1.167 | 14.527 | 6.655 | 1.00 | 40.97 |
| ATOM | 406 | CA | ASP | 1527 | 2.210 | 13.546 | 6.867 | 1.00 | 41.03 |
| ATOM | 407 | CB | ASP | 1527 | 3.497 | 14.235 | 7.316 | 1.00 | 45.30 |
| ATOM | 408 | CG | ASP | 1527 | 4.083 | 15.147 | 6.235 | 1.00 | 47.84 |
| ATOM | 409 | OD1 | ASP | 1527 | 3.700 | 15.041 | 5.047 | 1.00 | 48.84 |
| ATOM | 410 | OD2 | ASP | 1527 | 4.957 | 15.966 | 6.600 | 1.00 | 49.11 |

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ATOM     411  C   ASP  1527      1.782  12.485   7.858  1.00 39.01
ATOM     412  O   ASP  1527      2.021  11.298   7.651  1.00 40.04
ATOM     413  N   LEU  1528      1.094  12.917   8.909  1.00 35.93
ATOM     414  CA  LEU  1528      0.594  12.004   9.927  1.00 36.48
ATOM     415  CB  LEU  1528     -0.008  12.784  11.107  1.00 36.51
ATOM     416  CG  LEU  1528     -0.436  11.961  12.326  1.00 40.56
ATOM     417  CD1 LEU  1528      0.650  10.955  12.692  1.00 42.00
ATOM     418  CD2 LEU  1528     -0.770  12.877  13.499  1.00 38.25
ATOM     419  C   LEU  1528     -0.453  11.065   9.309  1.00 35.25
ATOM     420  O   LEU  1528     -0.442   9.855   9.566  1.00 36.37
ATOM     421  N   ILE  1529     -1.311  11.614   8.453  1.00 33.10
ATOM     422  CA  ILE  1529     -2.365  10.839   7.805  1.00 32.32
ATOM     423  CB  ILE  1529     -3.364  11.732   7.012  1.00 31.17
ATOM     424  CG2 ILE  1529     -4.311  10.861   6.187  1.00 32.01
ATOM     425  CG1 ILE  1529     -4.193  12.579   7.983  1.00 31.35
ATOM     426  CD1 ILE  1529     -5.024  13.662   7.335  1.00 32.59
ATOM     427  C   ILE  1529     -1.732   9.825   6.877  1.00 33.44
ATOM     428  O   ILE  1529     -2.148   8.667   6.860  1.00 35.41
ATOM     429  N   SER  1530     -0.733  10.269   6.108  1.00 33.40
ATOM     430  CA  SER  1530      0.007   9.414   5.171  1.00 34.34
ATOM     431  CB  SER  1530      1.126  10.197   4.495  1.00 38.37
ATOM     432  OG  SER  1530      0.605  11.332   3.835  1.00 46.02
ATOM     433  C   SER  1530      0.614   8.208   5.868  1.00 30.41
ATOM     434  O   SER  1530      0.494   7.083   5.376  1.00 30.50
ATOM     435  N   GLU  1531      1.256   8.449   7.010  1.00 27.40
ATOM     436  CA  GLU  1531      1.865   7.369   7.766  1.00 28.90
ATOM     437  CB  GLU  1531      2.629   7.907   8.973  1.00 28.45
ATOM     438  CG  GLU  1531      3.263   6.812   9.825  1.00 29.33
ATOM     439  CD  GLU  1531      4.094   7.344  10.979  1.00 31.14
ATOM     440  OE1 GLU  1531      4.913   6.561  11.495  1.00 33.14
ATOM     441  OE2 GLU  1531      3.940   8.522  11.378  1.00 31.11
ATOM     442  C   GLU  1531      0.824   6.351   8.215  1.00 30.88
ATOM     443  O   GLU  1531      1.118   5.146   8.259  1.00 32.35
ATOM     444  N   MET  1532     -0.377   6.832   8.553  1.00 29.86
ATOM     445  CA  MET  1532     -1.476   5.966   8.996  1.00 30.01
ATOM     446  CB  MET  1532     -2.608   6.800   9.596  1.00 29.58
ATOM     447  CG  MET  1532     -3.761   5.968  10.146  1.00 31.20
ATOM     448  SD  MET  1532     -5.095   6.973  10.779  1.00 29.37
ATOM     449  CE  MET  1532     -5.271   8.228   9.489  1.00 21.59
ATOM     450  C   MET  1532     -2.002   5.145   7.814  1.00 29.60
ATOM     451  O   MET  1532     -2.131   3.923   7.893  1.00 29.68
ATOM     452  N   GLU  1533     -2.257   5.824   6.702  1.00 30.38
ATOM     453  CA  GLU  1533     -2.755   5.176   5.495  1.00 30.12
ATOM     454  CB  GLU  1533     -2.987   6.221   4.423  1.00 25.79
ATOM     455  CG  GLU  1533     -4.117   7.154   4.784  1.00 26.67
ATOM     456  CD  GLU  1533     -5.420   6.405   5.064  1.00 29.90
ATOM     457  OE1 GLU  1533     -5.923   5.696   4.166  1.00 29.93
ATOM     458  OE2 GLU  1533     -5.939   6.518   6.197  1.00 29.10
ATOM     459  C   GLU  1533     -1.787   4.120   5.003  1.00 30.32
ATOM     460  O   GLU  1533     -2.197   3.043   4.563  1.00 32.06
ATOM     461  N   MET  1534     -0.500   4.435   5.136  1.00 29.97
ATOM     462  CA  MET  1534      0.606   3.571   4.737  1.00 31.22
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 463 | CB | MET | 1534 | 1.918 | 4.305 | 4.985 | 1.00 | 33.86 |
| ATOM | 464 | CG | MET | 1534 | 3.118 | 3.487 | 4.675 | 1.00 | 40.40 |
| ATOM | 465 | SD | MET | 1534 | 3.528 | 3.627 | 2.982 | 1.00 | 48.27 |
| ATOM | 466 | CE | MET | 1534 | 5.215 | 4.257 | 3.155 | 1.00 | 42.49 |
| ATOM | 467 | C | MET | 1534 | 0.565 | 2.304 | 5.581 | 1.00 | 30.90 |
| ATOM | 468 | O | MET | 1534 | 0.596 | 1.193 | 5.050 | 1.00 | 33.24 |
| ATOM | 469 | N | MET | 1535 | 0.493 | 2.485 | 6.896 | 1.00 | 29.07 |
| ATOM | 470 | CA | MET | 1535 | 0.417 | 1.354 | 7.813 | 1.00 | 28.82 |
| ATOM | 471 | CB | MET | 1535 | 0.325 | 1.829 | 9.274 | 1.00 | 28.87 |
| ATOM | 472 | CG | MET | 1535 | 1.622 | 2.434 | 9.803 | 1.00 | 28.16 |
| ATOM | 473 | SD | MET | 1535 | 1.674 | 2.633 | 11.595 | 1.00 | 30.96 |
| ATOM | 474 | CE | MET | 1535 | 1.393 | 4.335 | 11.729 | 1.00 | 27.69 |
| ATOM | 475 | C | MET | 1535 | -0.777 | 0.460 | 7.445 | 1.00 | 28.59 |
| ATOM | 476 | O | MET | 1535 | -0.682 | -0.774 | 7.530 | 1.00 | 30.37 |
| ATOM | 477 | N | LYS | 1536 | -1.885 | 1.072 | 7.019 | 1.00 | 26.53 |
| ATOM | 478 | CA | LYS | 1536 | -3.078 | 0.315 | 6.608 | 1.00 | 27.60 |
| ATOM | 479 | CB | LYS | 1536 | -4.237 | 1.253 | 6.283 | 1.00 | 25.88 |
| ATOM | 480 | CG | LYS | 1536 | -4.807 | 1.947 | 7.479 | 1.00 | 23.80 |
| ATOM | 481 | CD | LYS | 1536 | -5.925 | 2.857 | 7.061 | 1.00 | 21.64 |
| ATOM | 482 | CE | LYS | 1536 | -6.402 | 3.674 | 8.225 | 1.00 | 21.83 |
| ATOM | 483 | NZ | LYS | 1536 | -7.469 | 4.594 | 7.796 | 1.00 | 26.27 |
| ATOM | 484 | C | LYS | 1536 | -2.813 | -0.573 | 5.397 | 1.00 | 27.49 |
| ATOM | 485 | O | LYS | 1536 | -3.150 | -1.756 | 5.393 | 1.00 | 29.24 |
| ATOM | 486 | N | MET | 1537 | -2.186 | -0.014 | 4.372 | 1.00 | 27.89 |
| ATOM | 487 | CA | MET | 1537 | -1.890 | -0.783 | 3.172 | 1.00 | 29.12 |
| ATOM | 488 | CB | MET | 1537 | -1.321 | 0.136 | 2.085 | 1.00 | 32.72 |
| ATOM | 489 | CG | MET | 1537 | -2.282 | 1.208 | 1.566 | 1.00 | 37.18 |
| ATOM | 490 | SD | MET | 1537 | -3.740 | 0.505 | 0.744 | 1.00 | 43.17 |
| ATOM | 491 | CE | MET | 1537 | -2.964 | -0.152 | -0.698 | 1.00 | 43.04 |
| ATOM | 492 | C | MET | 1537 | -0.903 | -1.920 | 3.447 | 1.00 | 29.58 |
| ATOM | 493 | O | MET | 1537 | -1.102 | -3.049 | 2.996 | 1.00 | 27.53 |
| ATOM | 494 | N | ILE | 1538 | 0.142 | -1.626 | 4.223 | 1.00 | 28.64 |
| ATOM | 495 | CA | ILE | 1538 | 1.189 | -2.609 | 4.533 | 1.00 | 26.88 |
| ATOM | 496 | CB | ILE | 1538 | 2.381 | -1.948 | 5.280 | 1.00 | 25.23 |
| ATOM | 497 | CG2 | ILE | 1538 | 3.380 | -2.989 | 5.745 | 1.00 | 27.31 |
| ATOM | 498 | CG1 | ILE | 1538 | 3.097 | -0.968 | 4.345 | 1.00 | 22.70 |
| ATOM | 499 | CD1 | ILE | 1538 | 4.445 | -0.465 | 4.874 | 1.00 | 23.44 |
| ATOM | 500 | C | ILE | 1538 | 0.756 | -3.911 | 5.224 | 1.00 | 26.75 |
| ATOM | 501 | O | ILE | 1538 | 1.274 | -4.980 | 4.909 | 1.00 | 28.60 |
| ATOM | 502 | N | GLY | 1539 | -0.200 | -3.849 | 6.137 | 1.00 | 27.19 |
| ATOM | 503 | CA | GLY | 1539 | -0.625 | -5.069 | 6.812 | 1.00 | 26.88 |
| ATOM | 504 | C | GLY | 1539 | 0.207 | -5.369 | 8.039 | 1.00 | 26.04 |
| ATOM | 505 | O | GLY | 1539 | 1.220 | -4.708 | 8.281 | 1.00 | 27.96 |
| ATOM | 506 | N | LYS | 1540 | -0.195 | -6.396 | 8.788 | 1.00 | 23.25 |
| ATOM | 507 | CA | LYS | 1540 | 0.461 | -6.781 | 10.052 | 1.00 | 21.53 |
| ATOM | 508 | CB | LYS | 1540 | -0.573 | -7.350 | 11.028 | 1.00 | 20.48 |
| ATOM | 509 | CG | LYS | 1540 | -1.530 | -6.346 | 11.563 | 1.00 | 28.42 |
| ATOM | 510 | CD | LYS | 1540 | -2.542 | -6.977 | 12.502 | 1.00 | 36.24 |
| ATOM | 511 | CE | LYS | 1540 | -3.568 | -5.942 | 12.994 | 1.00 | 41.05 |
| ATOM | 512 | NZ | LYS | 1540 | -2.973 | -4.847 | 13.836 | 1.00 | 41.25 |
| ATOM | 513 | C | LYS | 1540 | 1.577 | -7.796 | 9.974 | 1.00 | 19.96 |
| ATOM | 514 | O | LYS | 1540 | 1.536 | -8.723 | 9.176 | 1.00 | 21.51 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 515 | N | HIS | 1541 | 2.514 | -7.670 | 10.905 | 1.00 | 19.82 |
| ATOM | 516 | CA | HIS | 1541 | 3.622 | -8.613 | 11.040 | 1.00 | 21.35 |
| ATOM | 517 | CB | HIS | 1541 | 4.704 | -8.411 | 9.972 | 1.00 | 21.39 |
| ATOM | 518 | CG | HIS | 1541 | 5.747 | -9.490 | 9.963 | 1.00 | 17.07 |
| ATOM | 519 | CD2 | HIS | 1541 | 5.810 | -10.667 | 9.292 | 1.00 | 18.04 |
| ATOM | 520 | ND1 | HIS | 1541 | 6.891 | -9.428 | 10.727 | 1.00 | 19.05 |
| ATOM | 521 | CE1 | HIS | 1541 | 7.609 | -10.522 | 10.535 | 1.00 | 19.63 |
| ATOM | 522 | NE2 | HIS | 1541 | 6.975 | -11.293 | 9.668 | 1.00 | 18.32 |
| ATOM | 523 | C | HIS | 1541 | 4.198 | -8.456 | 12.449 | 1.00 | 23.61 |
| ATOM | 524 | O | HIS | 1541 | 4.231 | -7.352 | 13.002 | 1.00 | 25.66 |
| ATOM | 525 | N | LYS | 1542 | 4.587 | -9.577 | 13.045 | 1.00 | 24.32 |
| ATOM | 526 | CA | LYS | 1542 | 5.141 | -9.610 | 14.396 | 1.00 | 27.04 |
| ATOM | 527 | CB | LYS | 1542 | 5.578 | -11.044 | 14.742 | 1.00 | 30.70 |
| ATOM | 528 | CG | LYS | 1542 | 6.130 | -11.239 | 16.150 | 1.00 | 40.75 |
| ATOM | 529 | CD | LYS | 1542 | 6.380 | -12.719 | 16.420 | 1.00 | 48.24 |
| ATOM | 530 | CE | LYS | 1542 | 6.995 | -13.414 | 15.183 | 1.00 | 56.89 |
| ATOM | 531 | NZ | LYS | 1542 | 7.457 | -14.831 | 15.421 | 1.00 | 60.99 |
| ATOM | 532 | C | LYS | 1542 | 6.318 | -8.674 | 14.608 | 1.00 | 24.59 |
| ATOM | 533 | O | LYS | 1542 | 6.462 | -8.067 | 15.676 | 1.00 | 23.35 |
| ATOM | 534 | N | ASN | 1543 | 7.147 | -8.546 | 13.576 | 1.00 | 22.05 |
| ATOM | 535 | CA | ASN | 1543 | 8.333 | -7.702 | 13.689 | 1.00 | 21.40 |
| ATOM | 536 | CB | ASN | 1543 | 9.558 | -8.482 | 13.217 | 1.00 | 20.89 |
| ATOM | 537 | CG | ASN | 1543 | 9.721 | -9.811 | 13.945 | 1.00 | 20.37 |
| ATOM | 538 | OD1 | ASN | 1543 | 9.501 | -10.883 | 13.372 | 1.00 | 24.97 |
| ATOM | 539 | ND2 | ASN | 1543 | 10.016 | -9.741 | 15.230 | 1.00 | 21.56 |
| ATOM | 540 | C | ASN | 1543 | 8.312 | -6.268 | 13.155 | 1.00 | 20.38 |
| ATOM | 541 | O | ASN | 1543 | 9.353 | -5.733 | 12.776 | 1.00 | 20.03 |
| ATOM | 542 | N | ILE | 1544 | 7.153 | -5.624 | 13.180 | 1.00 | 20.02 |
| ATOM | 543 | CA | ILE | 1544 | 7.037 | -4.226 | 12.771 | 1.00 | 21.14 |
| ATOM | 544 | CB | ILE | 1544 | 6.545 | -4.029 | 11.292 | 1.00 | 22.97 |
| ATOM | 545 | CG2 | ILE | 1544 | 7.436 | -4.810 | 10.334 | 1.00 | 23.27 |
| ATOM | 546 | CG1 | ILE | 1544 | 5.082 | -4.447 | 11.096 | 1.00 | 22.85 |
| ATOM | 547 | CD1 | ILE | 1544 | 4.485 | -3.974 | 9.760 | 1.00 | 18.94 |
| ATOM | 548 | C | ILE | 1544 | 6.044 | -3.590 | 13.757 | 1.00 | 20.02 |
| ATOM | 549 | O | ILE | 1544 | 5.342 | -4.309 | 14.466 | 1.00 | 21.00 |
| ATOM | 550 | N | ILE | 1545 | 6.103 | -2.275 | 13.943 | 1.00 | 20.09 |
| ATOM | 551 | CA | ILE | 1545 | 5.140 | -1.608 | 14.826 | 1.00 | 22.82 |
| ATOM | 552 | CB | ILE | 1545 | 5.586 | -0.161 | 15.198 | 1.00 | 23.07 |
| ATOM | 553 | CG2 | ILE | 1545 | 4.399 | 0.652 | 15.718 | 1.00 | 21.94 |
| ATOM | 554 | CG1 | ILE | 1545 | 6.759 | -0.178 | 16.193 | 1.00 | 20.49 |
| ATOM | 555 | CD1 | ILE | 1545 | 6.450 | -0.730 | 17.579 | 1.00 | 15.00 |
| ATOM | 556 | C | ILE | 1545 | 3.853 | -1.555 | 14.010 | 1.00 | 24.18 |
| ATOM | 557 | O | ILE | 1545 | 3.809 | -0.954 | 12.920 | 1.00 | 25.68 |
| ATOM | 558 | N | ASN | 1546 | 2.829 | -2.236 | 14.514 | 1.00 | 25.69 |
| ATOM | 559 | CA | ASN | 1546 | 1.528 | -2.311 | 13.853 | 1.00 | 24.23 |
| ATOM | 560 | CB | ASN | 1546 | 0.866 | -3.697 | 14.060 | 1.00 | 25.21 |
| ATOM | 561 | CG | ASN | 1546 | 1.690 | -4.834 | 13.481 | 1.00 | 21.10 |
| ATOM | 562 | OD1 | ASN | 1546 | 1.764 | -4.997 | 12.274 | 1.00 | 23.44 |
| ATOM | 563 | ND2 | ASN | 1546 | 2.324 | -5.606 | 14.343 | 1.00 | 18.20 |
| ATOM | 564 | C | ASN | 1546 | 0.567 | -1.235 | 14.325 | 1.00 | 23.12 |
| ATOM | 565 | O | ASN | 1546 | 0.709 | -0.682 | 15.426 | 1.00 | 24.14 |
| ATOM | 566 | N | LEU | 1547 | -0.382 | -0.920 | 13.456 | 1.00 | 23.49 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 567 | CA | LEU | 1547 | -1.417 | 0.069 | 13.718 | 1.00 | 24.50 |
| ATOM | 568 | CB | LEU | 1547 | -1.976 | 0.597 | 12.378 | 1.00 | 21.63 |
| ATOM | 569 | CG | LEU | 1547 | -3.189 | 1.535 | 12.353 | 1.00 | 22.37 |
| ATOM | 570 | CD1 | LEU | 1547 | -2.834 | 2.903 | 12.922 | 1.00 | 21.78 |
| ATOM | 571 | CD2 | LEU | 1547 | -3.714 | 1.660 | 10.930 | 1.00 | 21.31 |
| ATOM | 572 | C | LEU | 1547 | -2.510 | -0.681 | 14.495 | 1.00 | 26.70 |
| ATOM | 573 | O | LEU | 1547 | -2.849 | -1.823 | 14.160 | 1.00 | 28.96 |
| ATOM | 574 | N | LEU | 1548 | -3.017 | -0.082 | 15.565 | 1.00 | 25.96 |
| ATOM | 575 | CA | LEU | 1548 | -4.047 | -0.714 | 16.365 | 1.00 | 22.37 |
| ATOM | 576 | CB | LEU | 1548 | -3.686 | -0.682 | 17.868 | 1.00 | 17.76 |
| ATOM | 577 | CG | LEU | 1548 | -2.346 | -1.360 | 18.224 | 1.00 | 17.12 |
| ATOM | 578 | CD1 | LEU | 1548 | -2.150 | -1.468 | 19.708 | 1.00 | 18.81 |
| ATOM | 579 | CD2 | LEU | 1548 | -2.266 | -2.737 | 17.631 | 1.00 | 16.20 |
| ATOM | 580 | C | LEU | 1548 | -5.395 | -0.061 | 16.099 | 1.00 | 23.30 |
| ATOM | 581 | O | LEU | 1548 | -6.418 | -0.727 | 16.175 | 1.00 | 24.18 |
| ATOM | 582 | N | GLY | 1549 | -5.395 | 1.228 | 15.758 | 1.00 | 21.53 |
| ATOM | 583 | CA | GLY | 1549 | -6.636 | 1.933 | 15.485 | 1.00 | 22.47 |
| ATOM | 584 | C | GLY | 1549 | -6.392 | 3.421 | 15.340 | 1.00 | 24.62 |
| ATOM | 585 | O | GLY | 1549 | -5.245 | 3.835 | 15.163 | 1.00 | 25.06 |
| ATOM | 586 | N | ALA | 1550 | -7.459 | 4.219 | 15.409 | 1.00 | 24.15 |
| ATOM | 587 | CA | ALA | 1550 | -7.362 | 5.672 | 15.313 | 1.00 | 22.20 |
| ATOM | 588 | CB | ALA | 1550 | -7.063 | 6.079 | 13.890 | 1.00 | 19.97 |
| ATOM | 589 | C | ALA | 1550 | -8.602 | 6.415 | 15.802 | 1.00 | 23.75 |
| ATOM | 590 | O | ALA | 1550 | -9.707 | 5.876 | 15.804 | 1.00 | 26.43 |
| ATOM | 591 | N | CYS | 1551 | -8.383 | 7.660 | 16.213 | 1.00 | 25.34 |
| ATOM | 592 | CA | CYS | 1551 | -9.425 | 8.590 | 16.678 | 1.00 | 27.17 |
| ATOM | 593 | CB | CYS | 1551 | -9.160 | 9.045 | 18.127 | 1.00 | 26.84 |
| ATOM | 594 | SG | CYS | 1551 | -9.246 | 7.802 | 19.448 | 1.00 | 30.32 |
| ATOM | 595 | C | CYS | 1551 | -9.294 | 9.787 | 15.719 | 1.00 | 28.42 |
| ATOM | 596 | O | CYS | 1551 | -8.364 | 10.575 | 15.827 | 1.00 | 27.28 |
| ATOM | 597 | N | THR | 1552 | -10.145 | 9.823 | 14.702 | 1.00 | 30.47 |
| ATOM | 598 | CA | THR | 1552 | -10.076 | 10.873 | 13.690 | 1.00 | 30.58 |
| ATOM | 599 | CB | THR | 1552 | -10.061 | 10.219 | 12.280 | 1.00 | 30.58 |
| ATOM | 600 | OG1 | THR | 1552 | -11.266 | 9.465 | 12.096 | 1.00 | 31.11 |
| ATOM | 601 | CG2 | THR | 1552 | -8.895 | 9.255 | 12.151 | 1.00 | 27.59 |
| ATOM | 602 | C | THR | 1552 | -11.241 | 11.847 | 13.695 | 1.00 | 32.24 |
| ATOM | 603 | O | THR | 1552 | -11.192 | 12.911 | 13.070 | 1.00 | 28.56 |
| ATOM | 604 | N | GLN | 1553 | -12.339 | 11.408 | 14.286 | 1.00 | 35.46 |
| ATOM | 605 | CA | GLN | 1553 | -13.529 | 12.233 | 14.295 | 1.00 | 38.72 |
| ATOM | 606 | CB | GLN | 1553 | -14.775 | 11.359 | 14.148 | 1.00 | 38.66 |
| ATOM | 607 | CG | GLN | 1553 | -14.811 | 10.529 | 12.876 | 1.00 | 41.41 |
| ATOM | 608 | CD | GLN | 1553 | -14.695 | 11.381 | 11.627 | 1.00 | 44.05 |
| ATOM | 609 | OE1 | GLN | 1553 | -15.442 | 12.345 | 11.445 | 1.00 | 45.08 |
| ATOM | 610 | NE2 | GLN | 1553 | -13.746 | 11.033 | 10.765 | 1.00 | 43.32 |
| ATOM | 611 | C | GLN | 1553 | -13.658 | 13.168 | 15.483 | 1.00 | 41.20 |
| ATOM | 612 | O | GLN | 1553 | -13.230 | 12.837 | 16.590 | 1.00 | 39.89 |
| ATOM | 613 | N | ASP | 1554 | -14.225 | 14.344 | 15.219 | 1.00 | 44.03 |
| ATOM | 614 | CA | ASP | 1554 | -14.474 | 15.356 | 16.237 | 1.00 | 46.94 |
| ATOM | 615 | CB | ASP | 1554 | -15.778 | 15.028 | 16.976 | 1.00 | 49.94 |
| ATOM | 616 | CG | ASP | 1554 | -17.007 | 15.262 | 16.122 | 1.00 | 56.68 |
| ATOM | 617 | OD1 | ASP | 1554 | -17.966 | 15.878 | 16.631 | 1.00 | 64.76 |
| ATOM | 618 | OD2 | ASP | 1554 | -17.030 | 14.829 | 14.947 | 1.00 | 60.79 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 619 | C | ASP | 1554 | -13.343 | 15.563 | 17.244 | 1.00 | 47.24 |
| ATOM | 620 | O | ASP | 1554 | -13.522 | 15.375 | 18.452 | 1.00 | 48.98 |
| ATOM | 621 | N | GLY | 1555 | -12.182 | 15.966 | 16.747 | 1.00 | 44.00 |
| ATOM | 622 | CA | GLY | 1555 | -11.062 | 16.185 | 17.638 | 1.00 | 41.07 |
| ATOM | 623 | C | GLY | 1555 | -9.728 | 15.891 | 16.994 | 1.00 | 40.26 |
| ATOM | 624 | O | GLY | 1555 | -9.663 | 15.567 | 15.810 | 1.00 | 39.72 |
| ATOM | 625 | N | PRO | 1556 | -8.635 | 15.987 | 17.759 | 1.00 | 39.21 |
| ATOM | 626 | CD | PRO | 1556 | -8.634 | 16.266 | 19.208 | 1.00 | 39.09 |
| ATOM | 627 | CA | PRO | 1556 | -7.271 | 15.740 | 17.294 | 1.00 | 37.84 |
| ATOM | 628 | CB | PRO | 1556 | -6.436 | 15.947 | 18.549 | 1.00 | 39.66 |
| ATOM | 629 | CG | PRO | 1556 | -7.269 | 16.842 | 19.389 | 1.00 | 39.53 |
| ATOM | 630 | C | PRO | 1556 | -7.094 | 14.314 | 16.806 | 1.00 | 37.75 |
| ATOM | 631 | O | PRO | 1556 | -7.574 | 13.377 | 17.444 | 1.00 | 37.25 |
| ATOM | 632 | N | LEU | 1557 | -6.379 | 14.153 | 15.699 | 1.00 | 36.09 |
| ATOM | 633 | CA | LEU | 1557 | -6.112 | 12.844 | 15.124 | 1.00 | 34.69 |
| ATOM | 634 | CB | LEU | 1557 | -5.458 | 13.010 | 13.741 | 1.00 | 32.25 |
| ATOM | 635 | CG | LEU | 1557 | -4.962 | 11.774 | 12.972 | 1.00 | 31.23 |
| ATOM | 636 | CD1 | LEU | 1557 | -6.080 | 10.763 | 12.715 | 1.00 | 25.69 |
| ATOM | 637 | CD2 | LEU | 1557 | -4.339 | 12.219 | 11.669 | 1.00 | 28.21 |
| ATOM | 638 | C | LEU | 1557 | -5.190 | 12.057 | 16.060 | 1.00 | 34.59 |
| ATOM | 639 | O | LEU | 1557 | -4.173 | 12.578 | 16.524 | 1.00 | 32.09 |
| ATOM | 640 | N | TYR | 1558 | -5.606 | 10.841 | 16.396 | 1.00 | 32.63 |
| ATOM | 641 | CA | TYR | 1558 | -4.796 | 9.993 | 17.237 | 1.00 | 29.66 |
| ATOM | 642 | CB | TYR | 1558 | -5.529 | 9.630 | 18.534 | 1.00 | 33.14 |
| ATOM | 643 | CG | TYR | 1558 | -5.588 | 10.754 | 19.539 | 1.00 | 32.87 |
| ATOM | 644 | CD1 | TYR | 1558 | -6.583 | 10.793 | 20.517 | 1.00 | 34.58 |
| ATOM | 645 | CE1 | TYR | 1558 | -6.678 | 11.857 | 21.407 | 1.00 | 34.65 |
| ATOM | 646 | CD2 | TYR | 1558 | -4.678 | 11.805 | 19.483 | 1.00 | 35.69 |
| ATOM | 647 | CE2 | TYR | 1558 | -4.760 | 12.878 | 20.367 | 1.00 | 37.01 |
| ATOM | 648 | CZ | TYR | 1558 | -5.766 | 12.899 | 21.324 | 1.00 | 37.52 |
| ATOM | 649 | OH | TYR | 1558 | -5.868 | 13.986 | 22.164 | 1.00 | 40.19 |
| ATOM | 650 | C | TYR | 1558 | -4.529 | 8.747 | 16.436 | 1.00 | 28.08 |
| ATOM | 651 | O | TYR | 1558 | -5.467 | 8.137 | 15.924 | 1.00 | 30.12 |
| ATOM | 652 | N | VAL | 1559 | -3.254 | 8.444 | 16.225 | 1.00 | 25.89 |
| ATOM | 653 | CA | VAL | 1559 | -2.855 | 7.246 | 15.504 | 1.00 | 23.70 |
| ATOM | 654 | CB | VAL | 1559 | -1.729 | 7.528 | 14.485 | 1.00 | 23.78 |
| ATOM | 655 | CG1 | VAL | 1559 | -1.456 | 6.282 | 13.623 | 1.00 | 20.75 |
| ATOM | 656 | CG2 | VAL | 1559 | -2.101 | 8.738 | 13.604 | 1.00 | 22.54 |
| ATOM | 657 | C | VAL | 1559 | -2.358 | 6.311 | 16.596 | 1.00 | 23.47 |
| ATOM | 658 | O | VAL | 1559 | -1.328 | 6.572 | 17.220 | 1.00 | 26.84 |
| ATOM | 659 | N | ILE | 1560 | -3.146 | 5.283 | 16.889 | 1.00 | 23.58 |
| ATOM | 660 | CA | ILE | 1560 | -2.818 | 4.316 | 17.928 | 1.00 | 23.75 |
| ATOM | 661 | CB | ILE | 1560 | -4.112 | 3.732 | 18.552 | 1.00 | 22.67 |
| ATOM | 662 | CG2 | ILE | 1560 | -3.777 | 2.898 | 19.788 | 1.00 | 20.24 |
| ATOM | 663 | CG1 | ILE | 1560 | -5.063 | 4.884 | 18.904 | 1.00 | 20.09 |
| ATOM | 664 | CD1 | ILE | 1560 | -6.428 | 4.463 | 19.318 | 1.00 | 19.04 |
| ATOM | 665 | C | ILE | 1560 | -1.954 | 3.181 | 17.356 | 1.00 | 27.39 |
| ATOM | 666 | O | ILE | 1560 | -2.411 | 2.392 | 16.505 | 1.00 | 28.51 |
| ATOM | 667 | N | VAL | 1561 | -0.720 | 3.089 | 17.840 | 1.00 | 26.76 |
| ATOM | 668 | CA | VAL | 1561 | 0.238 | 2.088 | 17.368 | 1.00 | 25.91 |
| ATOM | 669 | CB | VAL | 1561 | 1.445 | 2.801 | 16.653 | 1.00 | 24.50 |
| ATOM | 670 | CG1 | VAL | 1561 | 0.952 | 3.480 | 15.397 | 1.00 | 13.55 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 671 | CG2 | VAL | 1561 | 2.054 | 3.870 | 17.551 | 1.00 | 20.39 |
| ATOM | 672 | C | VAL | 1561 | 0.693 | 1.151 | 18.519 | 1.00 | 24.80 |
| ATOM | 673 | O | VAL | 1561 | 0.397 | 1.417 | 19.696 | 1.00 | 25.26 |
| ATOM | 674 | N | GLU | 1562 | 1.349 | 0.032 | 18.192 | 1.00 | 22.30 |
| ATOM | 675 | CA | GLU | 1562 | 1.793 | -0.901 | 19.230 | 1.00 | 21.49 |
| ATOM | 676 | CB | GLU | 1562 | 2.369 | -2.179 | 18.630 | 1.00 | 16.65 |
| ATOM | 677 | CG | GLU | 1562 | 1.312 | -3.115 | 18.092 | 1.00 | 19.71 |
| ATOM | 678 | CD | GLU | 1562 | 1.895 | -4.356 | 17.460 | 1.00 | 21.58 |
| ATOM | 679 | OE1 | GLU | 1562 | 1.281 | -5.432 | 17.572 | 1.00 | 24.28 |
| ATOM | 680 | OE2 | GLU | 1562 | 2.956 | -4.260 | 16.825 | 1.00 | 23.74 |
| ATOM | 681 | C | GLU | 1562 | 2.802 | -0.261 | 20.158 | 1.00 | 23.56 |
| ATOM | 682 | O | GLU | 1562 | 3.581 | 0.578 | 19.738 | 1.00 | 24.82 |
| ATOM | 683 | N | TYR | 1563 | 2.787 | -0.665 | 21.422 | 1.00 | 26.96 |
| ATOM | 684 | CA | TYR | 1563 | 3.677 | -0.132 | 22.442 | 1.00 | 28.98 |
| ATOM | 685 | CB | TYR | 1563 | 2.907 | 0.035 | 23.744 | 1.00 | 30.34 |
| ATOM | 686 | CG | TYR | 1563 | 3.744 | 0.456 | 24.929 | 1.00 | 33.86 |
| ATOM | 687 | CD1 | TYR | 1563 | 4.457 | 1.653 | 24.915 | 1.00 | 36.58 |
| ATOM | 688 | CE1 | TYR | 1563 | 5.195 | 2.069 | 26.021 | 1.00 | 36.89 |
| ATOM | 689 | CD2 | TYR | 1563 | 3.787 | -0.322 | 26.082 | 1.00 | 34.25 |
| ATOM | 690 | CE2 | TYR | 1563 | 4.522 | 0.080 | 27.186 | 1.00 | 34.47 |
| ATOM | 691 | CZ | TYR | 1563 | 5.219 | 1.273 | 27.150 | 1.00 | 37.08 |
| ATOM | 692 | OH | TYR | 1563 | 5.965 | 1.662 | 28.228 | 1.00 | 44.10 |
| ATOM | 693 | C | TYR | 1563 | 4.884 | -1.043 | 22.668 | 1.00 | 30.53 |
| ATOM | 694 | O | TYR | 1563 | 4.745 | -2.269 | 22.751 | 1.00 | 30.66 |
| ATOM | 695 | N | ALA | 1564 | 6.068 | -0.440 | 22.779 | 1.00 | 31.09 |
| ATOM | 696 | CA | ALA | 1564 | 7.303 | -1.192 | 22.998 | 1.00 | 31.00 |
| ATOM | 697 | CB | ALA | 1564 | 8.236 | -1.026 | 21.792 | 1.00 | 30.82 |
| ATOM | 698 | C | ALA | 1564 | 7.940 | -0.663 | 24.283 | 1.00 | 29.32 |
| ATOM | 699 | O | ALA | 1564 | 8.703 | 0.309 | 24.274 | 1.00 | 32.26 |
| ATOM | 700 | N | SER | 1565 | 7.603 | -1.303 | 25.389 | 1.00 | 29.55 |
| ATOM | 701 | CA | SER | 1565 | 8.059 | -0.884 | 26.712 | 1.00 | 30.89 |
| ATOM | 702 | CB | SER | 1565 | 7.392 | -1.729 | 27.792 | 1.00 | 29.79 |
| ATOM | 703 | OG | SER | 1565 | 7.704 | -3.094 | 27.611 | 1.00 | 30.94 |
| ATOM | 704 | C | SER | 1565 | 9.547 | -0.840 | 26.986 | 1.00 | 31.39 |
| ATOM | 705 | O | SER | 1565 | 9.978 | -0.150 | 27.902 | 1.00 | 35.74 |
| ATOM | 706 | N | LYS | 1566 | 10.340 | -1.576 | 26.229 | 1.00 | 30.03 |
| ATOM | 707 | CA | LYS | 1566 | 11.756 | -1.560 | 26.495 | 1.00 | 28.80 |
| ATOM | 708 | CB | LYS | 1566 | 12.322 | -2.973 | 26.447 | 1.00 | 28.98 |
| ATOM | 709 | CG | LYS | 1566 | 11.756 | -3.842 | 27.563 | 1.00 | 25.35 |
| ATOM | 710 | CD | LYS | 1566 | 12.208 | -5.279 | 27.459 | 1.00 | 30.93 |
| ATOM | 711 | CE | LYS | 1566 | 11.875 | -6.001 | 28.747 | 1.00 | 31.41 |
| ATOM | 712 | NZ | LYS | 1566 | 12.315 | -7.421 | 28.716 | 1.00 | 32.83 |
| ATOM | 713 | C | LYS | 1566 | 12.529 | -0.595 | 25.623 | 1.00 | 29.93 |
| ATOM | 714 | O | LYS | 1566 | 13.756 | -0.672 | 25.544 | 1.00 | 30.89 |
| ATOM | 715 | N | GLY | 1567 | 11.799 | 0.322 | 24.979 | 1.00 | 30.67 |
| ATOM | 716 | CA | GLY | 1567 | 12.423 | 1.328 | 24.138 | 1.00 | 28.44 |
| ATOM | 717 | C | GLY | 1567 | 13.136 | 0.874 | 22.875 | 1.00 | 27.19 |
| ATOM | 718 | O | GLY | 1567 | 12.919 | -0.235 | 22.395 | 1.00 | 25.36 |
| ATOM | 719 | N | ASN | 1568 | 14.011 | 1.731 | 22.352 | 1.00 | 28.39 |
| ATOM | 720 | CA | ASN | 1568 | 14.735 | 1.421 | 21.130 | 1.00 | 28.41 |
| ATOM | 721 | CB | ASN | 1568 | 15.188 | 2.698 | 20.418 | 1.00 | 30.32 |
| ATOM | 722 | CG | ASN | 1568 | 16.396 | 3.352 | 21.058 | 1.00 | 33.42 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 723 | OD1 | ASN | 1568 | 17.418 | 2.720 | 21.317 | 1.00 | 35.16 |
| ATOM | 724 | ND2 | ASN | 1568 | 16.328 | 4.661 | 21.203 | 1.00 | 36.23 |
| ATOM | 725 | C | ASN | 1568 | 15.884 | 0.443 | 21.314 | 1.00 | 28.34 |
| ATOM | 726 | O | ASN | 1568 | 16.478 | 0.373 | 22.388 | 1.00 | 30.67 |
| ATOM | 727 | N | LEU | 1569 | 16.212 | -0.270 | 20.244 | 1.00 | 27.65 |
| ATOM | 728 | CA | LEU | 1569 | 17.269 | -1.270 | 20.247 | 1.00 | 29.10 |
| ATOM | 729 | CB | LEU | 1569 | 17.311 | -1.974 | 18.880 | 1.00 | 27.49 |
| ATOM | 730 | CG | LEU | 1569 | 18.292 | -3.130 | 18.657 | 1.00 | 28.82 |
| ATOM | 731 | CD1 | LEU | 1569 | 18.236 | -4.140 | 19.825 | 1.00 | 24.68 |
| ATOM | 732 | CD2 | LEU | 1569 | 17.994 | -3.791 | 17.316 | 1.00 | 22.26 |
| ATOM | 733 | C | LEU | 1569 | 18.667 | -0.790 | 20.676 | 1.00 | 29.37 |
| ATOM | 734 | O | LEU | 1569 | 19.389 | -1.525 | 21.355 | 1.00 | 29.72 |
| ATOM | 735 | N | ARG | 1570 | 19.058 | 0.425 | 20.303 | 1.00 | 30.89 |
| ATOM | 736 | CA | ARG | 1570 | 20.374 | 0.943 | 20.689 | 1.00 | 33.01 |
| ATOM | 737 | CB | ARG | 1570 | 20.591 | 2.353 | 20.121 | 1.00 | 30.95 |
| ATOM | 738 | CG | ARG | 1570 | 21.896 | 2.983 | 20.584 | 1.00 | 38.85 |
| ATOM | 739 | CD | ARG | 1570 | 21.968 | 4.472 | 20.303 | 1.00 | 43.03 |
| ATOM | 740 | NE | ARG | 1570 | 20.749 | 5.192 | 20.670 | 1.00 | 53.34 |
| ATOM | 741 | CZ | ARG | 1570 | 20.404 | 5.573 | 21.905 | 1.00 | 57.49 |
| ATOM | 742 | NH1 | ARG | 1570 | 21.184 | 5.310 | 22.955 | 1.00 | 55.59 |
| ATOM | 743 | NH2 | ARG | 1570 | 19.272 | 6.252 | 22.086 | 1.00 | 59.53 |
| ATOM | 744 | C | ARG | 1570 | 20.475 | 0.947 | 22.229 | 1.00 | 33.82 |
| ATOM | 745 | O | ARG | 1570 | 21.351 | 0.296 | 22.817 | 1.00 | 33.93 |
| ATOM | 746 | N | GLU | 1571 | 19.528 | 1.639 | 22.865 | 1.00 | 33.91 |
| ATOM | 747 | CA | GLU | 1571 | 19.435 | 1.746 | 24.317 | 1.00 | 32.59 |
| ATOM | 748 | CB | GLU | 1571 | 18.177 | 2.524 | 24.676 | 1.00 | 36.40 |
| ATOM | 749 | CG | GLU | 1571 | 18.174 | 3.958 | 24.175 | 1.00 | 45.91 |
| ATOM | 750 | CD | GLU | 1571 | 16.822 | 4.654 | 24.328 | 1.00 | 52.95 |
| ATOM | 751 | OE1 | GLU | 1571 | 15.793 | 3.959 | 24.529 | 1.00 | 54.50 |
| ATOM | 752 | OE2 | GLU | 1571 | 16.792 | 5.905 | 24.222 | 1.00 | 55.17 |
| ATOM | 753 | C | GLU | 1571 | 19.380 | 0.361 | 24.959 | 1.00 | 31.40 |
| ATOM | 754 | O | GLU | 1571 | 20.115 | 0.054 | 25.895 | 1.00 | 31.09 |
| ATOM | 755 | N | TYR | 1572 | 18.503 | -0.477 | 24.433 | 1.00 | 29.24 |
| ATOM | 756 | CA | TYR | 1572 | 18.334 | -1.835 | 24.920 | 1.00 | 27.43 |
| ATOM | 757 | CB | TYR | 1572 | 17.387 | -2.590 | 23.991 | 1.00 | 26.41 |
| ATOM | 758 | CG | TYR | 1572 | 17.196 | -4.045 | 24.311 | 1.00 | 23.13 |
| ATOM | 759 | CD1 | TYR | 1572 | 16.224 | -4.448 | 25.216 | 1.00 | 28.16 |
| ATOM | 760 | CE1 | TYR | 1572 | 15.983 | -5.784 | 25.456 | 1.00 | 28.32 |
| ATOM | 761 | CD2 | TYR | 1572 | 17.936 | -5.024 | 23.665 | 1.00 | 20.00 |
| ATOM | 762 | CE2 | TYR | 1572 | 17.699 | -6.361 | 23.899 | 1.00 | 22.28 |
| ATOM | 763 | CZ | TYR | 1572 | 16.721 | -6.731 | 24.801 | 1.00 | 26.53 |
| ATOM | 764 | OH | TYR | 1572 | 16.479 | -8.058 | 25.055 | 1.00 | 30.25 |
| ATOM | 765 | C | TYR | 1572 | 19.671 | -2.564 | 24.960 | 1.00 | 30.90 |
| ATOM | 766 | O | TYR | 1572 | 19.953 | -3.323 | 25.901 | 1.00 | 30.68 |
| ATOM | 767 | N | LEU | 1573 | 20.487 | -2.337 | 23.933 | 1.00 | 31.27 |
| ATOM | 768 | CA | LEU | 1573 | 21.776 | -2.995 | 23.841 | 1.00 | 33.33 |
| ATOM | 769 | CB | LEU | 1573 | 22.287 | -2.975 | 22.399 | 1.00 | 30.85 |
| ATOM | 770 | CG | LEU | 1573 | 21.643 | -3.908 | 21.370 | 1.00 | 26.92 |
| ATOM | 771 | CD1 | LEU | 1573 | 22.144 | -3.546 | 19.980 | 1.00 | 22.76 |
| ATOM | 772 | CD2 | LEU | 1573 | 21.939 | -5.372 | 21.695 | 1.00 | 25.82 |
| ATOM | 773 | C | LEU | 1573 | 22.801 | -2.390 | 24.791 | 1.00 | 36.07 |
| ATOM | 774 | O | LEU | 1573 | 23.544 | -3.117 | 25.457 | 1.00 | 36.40 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 775 | N | GLN | 1574 | 22.815 | -1.065 | 24.887 | 1.00 | 37.25 |
| ATOM | 776 | CA | GLN | 1574 | 23.763 | -0.391 | 25.759 | 1.00 | 37.41 |
| ATOM | 777 | CB | GLN | 1574 | 23.722 | 1.119 | 25.522 | 1.00 | 38.07 |
| ATOM | 778 | CG | GLN | 1574 | 24.240 | 1.529 | 24.147 | 1.00 | 40.76 |
| ATOM | 779 | CD | GLN | 1574 | 24.046 | 3.009 | 23.851 | 1.00 | 44.73 |
| ATOM | 780 | OE1 | GLN | 1574 | 23.391 | 3.740 | 24.597 | 1.00 | 46.47 |
| ATOM | 781 | NE2 | GLN | 1574 | 24.606 | 3.452 | 22.732 | 1.00 | 46.93 |
| ATOM | 782 | C | GLN | 1574 | 23.502 | -0.711 | 27.233 | 1.00 | 37.80 |
| ATOM | 783 | O | GLN | 1574 | 24.431 | -0.988 | 27.990 | 1.00 | 38.55 |
| ATOM | 784 | N | ALA | 1575 | 22.229 | -0.742 | 27.617 | 1.00 | 37.28 |
| ATOM | 785 | CA | ALA | 1575 | 21.846 | -1.021 | 28.987 | 1.00 | 35.47 |
| ATOM | 786 | CB | ALA | 1575 | 20.394 | -0.669 | 29.178 | 1.00 | 31.42 |
| ATOM | 787 | C | ALA | 1575 | 22.102 | -2.473 | 29.424 | 1.00 | 38.30 |
| ATOM | 788 | O | ALA | 1575 | 21.758 | -2.843 | 30.544 | 1.00 | 41.11 |
| ATOM | 789 | N | ARG | 1576 | 22.647 | -3.299 | 28.528 | 1.00 | 37.59 |
| ATOM | 790 | CA | ARG | 1576 | 22.943 | -4.687 | 28.869 | 1.00 | 37.23 |
| ATOM | 791 | CB | ARG | 1576 | 22.027 | -5.636 | 28.111 | 1.00 | 36.82 |
| ATOM | 792 | CG | ARG | 1576 | 20.599 | -5.481 | 28.561 | 1.00 | 34.61 |
| ATOM | 793 | CD | ARG | 1576 | 19.649 | -6.146 | 27.640 | 1.00 | 31.82 |
| ATOM | 794 | NE | ARG | 1576 | 18.308 | -6.147 | 28.201 | 1.00 | 31.54 |
| ATOM | 795 | CZ | ARG | 1576 | 17.590 | -5.051 | 28.426 | 1.00 | 33.71 |
| ATOM | 796 | NH1 | ARG | 1576 | 18.086 | -3.855 | 28.149 | 1.00 | 33.68 |
| ATOM | 797 | NH2 | ARG | 1576 | 16.337 | -5.160 | 28.857 | 1.00 | 38.97 |
| ATOM | 798 | C | ARG | 1576 | 24.405 | -5.052 | 28.683 | 1.00 | 38.53 |
| ATOM | 799 | O | ARG | 1576 | 24.790 | -6.231 | 28.700 | 1.00 | 38.39 |
| ATOM | 800 | N | ARG | 1577 | 25.226 | -4.017 | 28.538 | 1.00 | 39.28 |
| ATOM | 801 | CA | ARG | 1577 | 26.661 | -4.185 | 28.394 | 1.00 | 39.33 |
| ATOM | 802 | CB | ARG | 1577 | 27.306 | -2.855 | 27.998 | 1.00 | 35.44 |
| ATOM | 803 | CG | ARG | 1577 | 27.048 | -2.402 | 26.584 | 1.00 | 33.45 |
| ATOM | 804 | CD | ARG | 1577 | 27.696 | -1.042 | 26.330 | 1.00 | 32.83 |
| ATOM | 805 | NE | ARG | 1577 | 27.798 | -0.747 | 24.897 | 1.00 | 36.69 |
| ATOM | 806 | CZ | ARG | 1577 | 28.284 | 0.385 | 24.384 | 1.00 | 36.99 |
| ATOM | 807 | NH1 | ARG | 1577 | 28.719 | 1.359 | 25.175 | 1.00 | 40.35 |
| ATOM | 808 | NH2 | ARG | 1577 | 28.346 | 0.539 | 23.065 | 1.00 | 36.53 |
| ATOM | 809 | C | ARG | 1577 | 27.222 | -4.594 | 29.754 | 1.00 | 41.24 |
| ATOM | 810 | O | ARG | 1577 | 26.652 | -4.244 | 30.796 | 1.00 | 41.03 |
| ATOM | 811 | N | PRO | 1578 | 28.307 | -5.381 | 29.769 | 1.00 | 44.39 |
| ATOM | 812 | CD | PRO | 1578 | 29.038 | -6.041 | 28.667 | 1.00 | 44.50 |
| ATOM | 813 | CA | PRO | 1578 | 28.877 | -5.766 | 31.066 | 1.00 | 44.89 |
| ATOM | 814 | CB | PRO | 1578 | 29.933 | -6.809 | 30.686 | 1.00 | 42.49 |
| ATOM | 815 | CG | PRO | 1578 | 30.352 | -6.391 | 29.327 | 1.00 | 43.63 |
| ATOM | 816 | C | PRO | 1578 | 29.490 | -4.493 | 31.672 | 1.00 | 45.20 |
| ATOM | 817 | O | PRO | 1578 | 29.814 | -3.538 | 30.947 | 1.00 | 44.68 |
| ATOM | 818 | N | PRO | 1579 | 29.604 | -4.432 | 33.003 | 1.00 | 46.51 |
| ATOM | 819 | CD | PRO | 1579 | 29.208 | -5.463 | 33.981 | 1.00 | 46.36 |
| ATOM | 820 | CA | PRO | 1579 | 30.169 | -3.265 | 33.685 | 1.00 | 47.56 |
| ATOM | 821 | CB | PRO | 1579 | 30.175 | -3.708 | 35.141 | 1.00 | 46.45 |
| ATOM | 822 | CG | PRO | 1579 | 28.997 | -4.638 | 35.205 | 1.00 | 47.51 |
| ATOM | 823 | C | PRO | 1579 | 31.575 | -2.904 | 33.200 | 1.00 | 50.19 |
| ATOM | 824 | O | PRO | 1579 | 32.481 | -3.739 | 33.196 | 1.00 | 53.53 |
| ATOM | 825 | N | ALA | 1592 | 19.097 | -5.342 | 32.478 | 1.00 | 60.30 |
| ATOM | 826 | CA | ALA | 1592 | 20.535 | -5.076 | 32.445 | 1.00 | 59.47 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 827 | CB | ALA | 1592 | 20.975 | -4.338 | 33.715 | 1.00 | 61.58 |
| ATOM | 828 | C | ALA | 1592 | 21.367 | -6.350 | 32.252 | 1.00 | 58.15 |
| ATOM | 829 | O | ALA | 1592 | 22.543 | -6.285 | 31.879 | 1.00 | 59.09 |
| ATOM | 830 | N | ALA | 1593 | 20.754 | -7.510 | 32.479 | 1.00 | 55.79 |
| ATOM | 831 | CA | ALA | 1593 | 21.457 | -8.775 | 32.324 | 1.00 | 55.06 |
| ATOM | 832 | CB | ALA | 1593 | 20.519 | -9.939 | 32.604 | 1.00 | 57.05 |
| ATOM | 833 | C | ALA | 1593 | 22.053 | -8.897 | 30.924 | 1.00 | 53.57 |
| ATOM | 834 | O | ALA | 1593 | 21.402 | -8.598 | 29.926 | 1.00 | 53.85 |
| ATOM | 835 | N | GLN | 1594 | 23.303 | -9.336 | 30.862 | 1.00 | 53.22 |
| ATOM | 836 | CA | GLN | 1594 | 24.004 | -9.490 | 29.599 | 1.00 | 50.13 |
| ATOM | 837 | CB | GLN | 1594 | 25.400 | -10.082 | 29.832 | 1.00 | 50.73 |
| ATOM | 838 | CG | GLN | 1594 | 26.308 | -9.253 | 30.743 | 1.00 | 54.69 |
| ATOM | 839 | CD | GLN | 1594 | 27.550 | -10.019 | 31.217 | 1.00 | 57.79 |
| ATOM | 840 | OE1 | GLN | 1594 | 28.075 | -10.900 | 30.524 | 1.00 | 58.82 |
| ATOM | 841 | NE2 | GLN | 1594 | 28.026 | -9.673 | 32.407 | 1.00 | 59.53 |
| ATOM | 842 | C | GLN | 1594 | 23.210 | -10.374 | 28.637 | 1.00 | 47.73 |
| ATOM | 843 | O | GLN | 1594 | 22.427 | -11.241 | 29.054 | 1.00 | 47.09 |
| ATOM | 844 | N | LEU | 1595 | 23.418 | -10.133 | 27.350 | 1.00 | 45.64 |
| ATOM | 845 | CA | LEU | 1595 | 22.758 | -10.880 | 26.292 | 1.00 | 42.00 |
| ATOM | 846 | CB | LEU | 1595 | 22.405 | -9.947 | 25.122 | 1.00 | 37.98 |
| ATOM | 847 | CG | LEU | 1595 | 21.345 | -8.894 | 25.446 | 1.00 | 37.70 |
| ATOM | 848 | CD1 | LEU | 1595 | 21.568 | -7.611 | 24.660 | 1.00 | 33.34 |
| ATOM | 849 | CD2 | LEU | 1595 | 19.971 | -9.479 | 25.222 | 1.00 | 32.84 |
| ATOM | 850 | C | LEU | 1595 | 23.729 | -11.944 | 25.828 | 1.00 | 40.92 |
| ATOM | 851 | O | LEU | 1595 | 24.944 | -11.745 | 25.855 | 1.00 | 41.12 |
| ATOM | 852 | N | SER | 1596 | 23.201 | -13.103 | 25.471 | 1.00 | 40.09 |
| ATOM | 853 | CA | SER | 1596 | 24.044 | -14.178 | 24.985 | 1.00 | 38.93 |
| ATOM | 854 | CB | SER | 1596 | 23.388 | -15.535 | 25.235 | 1.00 | 37.45 |
| ATOM | 855 | OG | SER | 1596 | 22.158 | -15.662 | 24.545 | 1.00 | 39.49 |
| ATOM | 856 | C | SER | 1596 | 24.302 | -13.987 | 23.499 | 1.00 | 39.41 |
| ATOM | 857 | O | SER | 1596 | 23.634 | -13.183 | 22.832 | 1.00 | 39.51 |
| ATOM | 858 | N | SER | 1597 | 25.266 | -14.738 | 22.977 | 1.00 | 39.17 |
| ATOM | 859 | CA | SER | 1597 | 25.587 | -14.667 | 21.563 | 1.00 | 40.23 |
| ATOM | 860 | CB | SER | 1597 | 26.740 | -15.611 | 21.230 | 1.00 | 39.96 |
| ATOM | 861 | OG | SER | 1597 | 27.865 | -15.339 | 22.048 | 1.00 | 46.60 |
| ATOM | 862 | C | SER | 1597 | 24.347 | -15.057 | 20.773 | 1.00 | 39.65 |
| ATOM | 863 | O | SER | 1597 | 24.066 | -14.469 | 19.725 | 1.00 | 41.13 |
| ATOM | 864 | N | LYS | 1598 | 23.590 | -16.023 | 21.291 | 1.00 | 36.82 |
| ATOM | 865 | CA | LYS | 1598 | 22.390 | -16.467 | 20.611 | 1.00 | 36.17 |
| ATOM | 866 | CB | LYS | 1598 | 21.827 | -17.742 | 21.217 | 1.00 | 36.19 |
| ATOM | 867 | CG | LYS | 1598 | 21.030 | -18.562 | 20.180 | 1.00 | 39.59 |
| ATOM | 868 | CD | LYS | 1598 | 20.150 | -19.623 | 20.830 | 1.00 | 37.49 |
| ATOM | 869 | CE | LYS | 1598 | 19.769 | -20.719 | 19.855 | 1.00 | 39.64 |
| ATOM | 870 | NZ | LYS | 1598 | 20.976 | -21.437 | 19.380 | 1.00 | 41.43 |
| ATOM | 871 | C | LYS | 1598 | 21.340 | -15.381 | 20.649 | 1.00 | 37.72 |
| ATOM | 872 | O | LYS | 1598 | 20.604 | -15.213 | 19.677 | 1.00 | 39.82 |
| ATOM | 873 | N | ASP | 1599 | 21.291 | -14.627 | 21.752 | 1.00 | 36.20 |
| ATOM | 874 | CA | ASP | 1599 | 20.331 | -13.530 | 21.907 | 1.00 | 33.96 |
| ATOM | 875 | CB | ASP | 1599 | 20.456 | -12.884 | 23.279 | 1.00 | 35.66 |
| ATOM | 876 | CG | ASP | 1599 | 19.913 | -13.744 | 24.394 | 1.00 | 36.18 |
| ATOM | 877 | OD1 | ASP | 1599 | 20.365 | -13.565 | 25.544 | 1.00 | 39.14 |
| ATOM | 878 | OD2 | ASP | 1599 | 19.036 | -14.593 | 24.128 | 1.00 | 33.40 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 879 | C | ASP | 1599 | 20.595 | -12.471 | 20.857 | 1.00 | 33.57 |
| ATOM | 880 | O | ASP | 1599 | 19.660 | -11.953 | 20.225 | 1.00 | 32.60 |
| ATOM | 881 | N | LEU | 1600 | 21.871 | -12.123 | 20.706 | 1.00 | 32.82 |
| ATOM | 882 | CA | LEU | 1600 | 22.304 | -11.121 | 19.735 | 1.00 | 31.14 |
| ATOM | 883 | CB | LEU | 1600 | 23.804 | -10.850 | 19.916 | 1.00 | 30.23 |
| ATOM | 884 | CG | LEU | 1600 | 24.174 | -10.153 | 21.242 | 1.00 | 27.52 |
| ATOM | 885 | CD1 | LEU | 1600 | 25.660 | -9.877 | 21.324 | 1.00 | 24.11 |
| ATOM | 886 | CD2 | LEU | 1600 | 23.408 | -8.857 | 21.369 | 1.00 | 21.94 |
| ATOM | 887 | C | LEU | 1600 | 21.964 | -11.523 | 18.291 | 1.00 | 29.24 |
| ATOM | 888 | O | LEU | 1600 | 21.385 | -10.734 | 17.541 | 1.00 | 27.61 |
| ATOM | 889 | N | VAL | 1601 | 22.271 | -12.764 | 17.930 | 1.00 | 27.38 |
| ATOM | 890 | CA | VAL | 1601 | 21.983 | -13.268 | 16.597 | 1.00 | 27.26 |
| ATOM | 891 | CB | VAL | 1601 | 22.648 | -14.649 | 16.345 | 1.00 | 30.47 |
| ATOM | 892 | CG1 | VAL | 1601 | 22.403 | -15.104 | 14.921 | 1.00 | 28.72 |
| ATOM | 893 | CG2 | VAL | 1601 | 24.156 | -14.568 | 16.593 | 1.00 | 29.92 |
| ATOM | 894 | C | VAL | 1601 | 20.474 | -13.353 | 16.399 | 1.00 | 26.23 |
| ATOM | 895 | O | VAL | 1601 | 19.991 | -13.147 | 15.295 | 1.00 | 25.54 |
| ATOM | 896 | N | SER | 1602 | 19.733 | -13.590 | 17.478 | 1.00 | 27.43 |
| ATOM | 897 | CA | SER | 1602 | 18.277 | -13.671 | 17.406 | 1.00 | 27.09 |
| ATOM | 898 | CB | SER | 1602 | 17.731 | -14.259 | 18.694 | 1.00 | 29.02 |
| ATOM | 899 | OG | SER | 1602 | 16.317 | -14.306 | 18.646 | 1.00 | 35.77 |
| ATOM | 900 | C | SER | 1602 | 17.669 | -12.280 | 17.149 | 1.00 | 26.87 |
| ATOM | 901 | O | SER | 1602 | 16.643 | -12.141 | 16.465 | 1.00 | 25.13 |
| ATOM | 902 | N | CYS | 1603 | 18.289 | -11.262 | 17.737 | 1.00 | 26.09 |
| ATOM | 903 | CA | CYS | 1603 | 17.878 | -9.871 | 17.561 | 1.00 | 24.81 |
| ATOM | 904 | CB | CYS | 1603 | 18.797 | -8.937 | 18.350 | 1.00 | 23.87 |
| ATOM | 905 | SG | CYS | 1603 | 18.512 | -7.186 | 18.059 | 0.50 | 24.17 |
| ATOM | 906 | C | CYS | 1603 | 17.994 | -9.517 | 16.090 | 1.00 | 25.24 |
| ATOM | 907 | O | CYS | 1603 | 17.083 | -8.932 | 15.520 | 1.00 | 27.48 |
| ATOM | 908 | N | ALA | 1604 | 19.138 | -9.854 | 15.492 | 1.00 | 26.80 |
| ATOM | 909 | CA | ALA | 1604 | 19.422 | -9.592 | 14.073 | 1.00 | 26.15 |
| ATOM | 910 | CB | ALA | 1604 | 20.851 | -10.035 | 13.741 | 1.00 | 24.35 |
| ATOM | 911 | C | ALA | 1604 | 18.419 | -10.302 | 13.168 | 1.00 | 26.61 |
| ATOM | 912 | O | ALA | 1604 | 17.894 | -9.713 | 12.226 | 1.00 | 28.81 |
| ATOM | 913 | N | TYR | 1605 | 18.130 | -11.557 | 13.488 | 1.00 | 27.10 |
| ATOM | 914 | CA | TYR | 1605 | 17.175 | -12.359 | 12.730 | 1.00 | 27.02 |
| ATOM | 915 | CB | TYR | 1605 | 17.104 | -13.751 | 13.334 | 1.00 | 27.35 |
| ATOM | 916 | CG | TYR | 1605 | 15.997 | -14.608 | 12.789 | 1.00 | 31.67 |
| ATOM | 917 | CD1 | TYR | 1605 | 16.109 | -15.244 | 11.546 | 1.00 | 32.96 |
| ATOM | 918 | CE1 | TYR | 1605 | 15.069 | -16.049 | 11.053 | 1.00 | 29.27 |
| ATOM | 919 | CD2 | TYR | 1605 | 14.830 | -14.797 | 13.520 | 1.00 | 31.42 |
| ATOM | 920 | CE2 | TYR | 1605 | 13.801 | -15.596 | 13.038 | 1.00 | 28.20 |
| ATOM | 921 | CZ | TYR | 1605 | 13.922 | -16.212 | 11.810 | 1.00 | 29.20 |
| ATOM | 922 | OH | TYR | 1605 | 12.855 | -16.944 | 11.364 | 1.00 | 27.90 |
| ATOM | 923 | C | TYR | 1605 | 15.766 | -11.735 | 12.658 | 1.00 | 27.90 |
| ATOM | 924 | O | TYR | 1605 | 15.180 | -11.635 | 11.578 | 1.00 | 28.40 |
| ATOM | 925 | N | GLN | 1606 | 15.231 | -11.319 | 13.807 | 1.00 | 27.12 |
| ATOM | 926 | CA | GLN | 1606 | 13.907 | -10.699 | 13.892 | 1.00 | 25.32 |
| ATOM | 927 | CB | GLN | 1606 | 13.561 | -10.383 | 15.342 | 1.00 | 24.31 |
| ATOM | 928 | CG | GLN | 1606 | 13.329 | -11.608 | 16.210 | 1.00 | 25.05 |
| ATOM | 929 | CD | GLN | 1606 | 13.052 | -11.243 | 17.649 | 1.00 | 26.35 |
| ATOM | 930 | OE1 | GLN | 1606 | 12.087 | -10.542 | 17.944 | 1.00 | 26.11 |

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ATOM     931  NE2 GLN  1606       13.917 -11.684  18.551  1.00 27.77
ATOM     932  C   GLN  1606       13.849  -9.415  13.078  1.00 27.52
ATOM     933  O   GLN  1606       12.825  -9.089  12.455  1.00 27.87
ATOM     934  N   VAL  1607       14.943  -8.662  13.122  1.00 27.90
ATOM     935  CA  VAL  1607       15.053  -7.419  12.359  1.00 26.41
ATOM     936  CB  VAL  1607       16.337  -6.661  12.731  1.00 25.61
ATOM     937  CG1 VAL  1607       16.545  -5.457  11.800  1.00 27.37
ATOM     938  CG2 VAL  1607       16.277  -6.224  14.190  1.00 21.50
ATOM     939  C   VAL  1607       15.035  -7.718  10.860  1.00 26.09
ATOM     940  O   VAL  1607       14.337  -7.046  10.096  1.00 28.48
ATOM     941  N   ALA  1608       15.795  -8.722  10.435  1.00 23.05
ATOM     942  CA  ALA  1608       15.812  -9.079   9.027  1.00 20.32
ATOM     943  CB  ALA  1608       16.823 -10.145   8.783  1.00 14.95
ATOM     944  C   ALA  1608       14.418  -9.558   8.600  1.00 23.08
ATOM     945  O   ALA  1608       14.033  -9.405   7.432  1.00 23.91
ATOM     946  N   ARG  1609       13.671 -10.169   9.530  1.00 24.57
ATOM     947  CA  ARG  1609       12.314 -10.628   9.246  1.00 24.30
ATOM     948  CB  ARG  1609       11.822 -11.577  10.326  1.00 26.13
ATOM     949  CG  ARG  1609       12.278 -12.979  10.114  1.00 31.07
ATOM     950  CD  ARG  1609       11.449 -13.885  10.939  1.00 36.13
ATOM     951  NE  ARG  1609       10.771 -14.865  10.115  1.00 38.37
ATOM     952  CZ  ARG  1609        9.931 -15.778  10.594  1.00 37.95
ATOM     953  NH1 ARG  1609        9.674 -15.828  11.898  1.00 35.31
ATOM     954  NH2 ARG  1609        9.353 -16.649   9.776  1.00 37.85
ATOM     955  C   ARG  1609       11.318  -9.490   9.065  1.00 22.34
ATOM     956  O   ARG  1609       10.470  -9.542   8.160  1.00 24.57
ATOM     957  N   GLY  1610       11.375  -8.500   9.948  1.00 20.52
ATOM     958  CA  GLY  1610       10.497  -7.353   9.827  1.00 19.33
ATOM     959  C   GLY  1610       10.732  -6.715   8.464  1.00 20.04
ATOM     960  O   GLY  1610        9.794  -6.455   7.693  1.00 19.10
ATOM     961  N   MET  1611       12.011  -6.545   8.130  1.00 18.21
ATOM     962  CA  MET  1611       12.423  -5.970   6.851  1.00 20.32
ATOM     963  CB  MET  1611       13.925  -5.737   6.838  1.00 19.20
ATOM     964  CG  MET  1611       14.371  -4.547   7.694  1.00 20.83
ATOM     965  SD  MET  1611       13.449  -2.960   7.422  1.00 25.39
ATOM     966  CE  MET  1611       13.869  -2.525   5.757  1.00 18.67
ATOM     967  C   MET  1611       12.024  -6.843   5.670  1.00 23.98
ATOM     968  O   MET  1611       11.608  -6.332   4.613  1.00 24.13
ATOM     969  N   GLU  1612       12.141  -8.162   5.825  1.00 25.76
ATOM     970  CA  GLU  1612       11.759  -9.059   4.743  1.00 25.49
ATOM     971  CB  GLU  1612       11.980 -10.522   5.110  1.00 26.09
ATOM     972  CG  GLU  1612       11.587 -11.468   3.968  1.00 26.56
ATOM     973  CD  GLU  1612       11.735 -12.942   4.313  1.00 29.26
ATOM     974  OE1 GLU  1612       11.386 -13.316   5.448  1.00 29.10
ATOM     975  OE2 GLU  1612       12.190 -13.725   3.443  1.00 31.11
ATOM     976  C   GLU  1612       10.283  -8.821   4.398  1.00 26.29
ATOM     977  O   GLU  1612        9.916  -8.728   3.226  1.00 28.46
ATOM     978  N   TYR  1613        9.437  -8.700   5.422  1.00 24.78
ATOM     979  CA  TYR  1613        8.003  -8.456   5.212  1.00 23.07
ATOM     980  CB  TYR  1613        7.263  -8.526   6.549  1.00 23.75
ATOM     981  CG  TYR  1613        5.785  -8.218   6.449  1.00 20.80
ATOM     982  CD1 TYR  1613        4.880  -9.213   6.062  1.00 20.97
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ATOM    983  CE1 TYR  1613     3.517  -8.944   5.958  1.00 20.03
ATOM    984  CD2 TYR  1613     5.289  -6.938   6.731  1.00 19.72
ATOM    985  CE2 TYR  1613     3.926  -6.661   6.628  1.00 21.87
ATOM    986  CZ  TYR  1613     3.046  -7.672   6.244  1.00 24.87
ATOM    987  OH  TYR  1613     1.694  -7.420   6.161  1.00 24.37
ATOM    988  C   TYR  1613     7.766  -7.094   4.550  1.00 21.68
ATOM    989  O   TYR  1613     6.970  -6.979   3.615  1.00 20.20
ATOM    990  N   LEU  1614     8.436  -6.065   5.062  1.00 21.72
ATOM    991  CA  LEU  1614     8.321  -4.713   4.519  1.00 20.42
ATOM    992  CB  LEU  1614     9.169  -3.747   5.350  1.00 17.68
ATOM    993  CG  LEU  1614     8.607  -3.395   6.733  1.00 18.47
ATOM    994  CD1 LEU  1614     9.504  -2.425   7.470  1.00 16.59
ATOM    995  CD2 LEU  1614     7.230  -2.795   6.558  1.00 14.07
ATOM    996  C   LEU  1614     8.729  -4.676   3.043  1.00 21.70
ATOM    997  O   LEU  1614     8.073  -4.038   2.211  1.00 22.25
ATOM    998  N   ALA  1615     9.819  -5.366   2.729  1.00 21.55
ATOM    999  CA  ALA  1615    10.313  -5.435   1.355  1.00 20.52
ATOM   1000  CB  ALA  1615    11.625  -6.207   1.292  1.00 19.78
ATOM   1001  C   ALA  1615     9.264  -6.098   0.491  1.00 19.98
ATOM   1002  O   ALA  1615     8.945  -5.587  -0.579  1.00 20.14
ATOM   1003  N   SER  1616     8.692  -7.205   0.972  1.00 20.65
ATOM   1004  CA  SER  1616     7.660  -7.919   0.207  1.00 19.59
ATOM   1005  CB  SER  1616     7.283  -9.217   0.912  1.00 15.96
ATOM   1006  OG  SER  1616     6.415  -8.966   2.007  1.00 16.62
ATOM   1007  C   SER  1616     6.397  -7.062  -0.018  1.00 22.05
ATOM   1008  O   SER  1616     5.650  -7.266  -0.975  1.00 23.62
ATOM   1009  N   LYS  1617     6.136  -6.135   0.895  1.00 23.39
ATOM   1010  CA  LYS  1617     4.997  -5.237   0.779  1.00 23.02
ATOM   1011  CB  LYS  1617     4.436  -4.881   2.160  1.00 21.50
ATOM   1012  CG  LYS  1617     3.709  -6.046   2.851  1.00 24.94
ATOM   1013  CD  LYS  1617     2.463  -6.448   2.059  1.00 26.57
ATOM   1014  CE  LYS  1617     1.691  -7.571   2.725  1.00 31.05
ATOM   1015  NZ  LYS  1617     2.401  -8.852   2.601  1.00 38.73
ATOM   1016  C   LYS  1617     5.346  -3.981  -0.017  1.00 24.01
ATOM   1017  O   LYS  1617     4.588  -3.007  -0.013  1.00 28.15
ATOM   1018  N   LYS  1618     6.496  -4.002  -0.679  1.00 23.84
ATOM   1019  CA  LYS  1618     6.957  -2.883  -1.528  1.00 24.05
ATOM   1020  CB  LYS  1618     5.871  -2.513  -2.555  1.00 25.74
ATOM   1021  CG  LYS  1618     5.734  -3.465  -3.749  1.00 28.34
ATOM   1022  CD  LYS  1618     5.557  -4.914  -3.328  1.00 32.45
ATOM   1023  CE  LYS  1618     5.590  -5.850  -4.520  1.00 30.41
ATOM   1024  NZ  LYS  1618     4.373  -5.748  -5.354  1.00 31.84
ATOM   1025  C   LYS  1618     7.404  -1.610  -0.796  1.00 23.84
ATOM   1026  O   LYS  1618     7.533  -0.548  -1.402  1.00 20.60
ATOM   1027  N   CYS  1619     7.719  -1.744   0.489  1.00 25.11
ATOM   1028  CA  CYS  1619     8.103  -0.614   1.312  1.00 21.68
ATOM   1029  CB  CYS  1619     7.338  -0.690   2.643  1.00 20.84
ATOM   1030  SG  CYS  1619     7.916   0.427   3.957  1.00 26.69
ATOM   1031  C   CYS  1619     9.586  -0.480   1.543  1.00 23.16
ATOM   1032  O   CYS  1619    10.257  -1.435   1.958  1.00 25.60
ATOM   1033  N   ILE  1620    10.110   0.717   1.288  1.00 23.91
ATOM   1034  CA  ILE  1620    11.532   1.046   1.474  1.00 26.01
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1035 | CB | ILE | 1620 | 12.098 | 1.830 | 0.236 | 1.00 | 22.61 |
| ATOM | 1036 | CG2 | ILE | 1620 | 13.551 | 2.259 | 0.471 | 1.00 | 16.86 |
| ATOM | 1037 | CG1 | ILE | 1620 | 12.014 | 0.977 | -1.026 | 1.00 | 22.72 |
| ATOM | 1038 | CD1 | ILE | 1620 | 12.096 | 1.804 | -2.316 | 1.00 | 23.62 |
| ATOM | 1039 | C | ILE | 1620 | 11.566 | 1.934 | 2.729 | 1.00 | 26.83 |
| ATOM | 1040 | O | ILE | 1620 | 10.900 | 2.965 | 2.772 | 1.00 | 28.92 |
| ATOM | 1041 | N | HIS | 1621 | 12.293 | 1.500 | 3.758 | 1.00 | 26.44 |
| ATOM | 1042 | CA | HIS | 1621 | 12.386 | 2.245 | 5.007 | 1.00 | 23.61 |
| ATOM | 1043 | CB | HIS | 1621 | 13.142 | 1.429 | 6.065 | 1.00 | 20.98 |
| ATOM | 1044 | CG | HIS | 1621 | 12.940 | 1.917 | 7.463 | 1.00 | 21.57 |
| ATOM | 1045 | CD2 | HIS | 1621 | 12.321 | 1.346 | 8.528 | 1.00 | 20.74 |
| ATOM | 1046 | ND1 | HIS | 1621 | 13.382 | 3.151 | 7.897 | 1.00 | 21.08 |
| ATOM | 1047 | CE1 | HIS | 1621 | 13.035 | 3.321 | 9.162 | 1.00 | 21.00 |
| ATOM | 1048 | NE2 | HIS | 1621 | 12.396 | 2.237 | 9.572 | 1.00 | 21.97 |
| ATOM | 1049 | C | HIS | 1621 | 13.054 | 3.582 | 4.841 | 1.00 | 24.83 |
| ATOM | 1050 | O | HIS | 1621 | 12.560 | 4.585 | 5.310 | 1.00 | 25.76 |
| ATOM | 1051 | N | ARG | 1622 | 14.247 | 3.565 | 4.269 | 1.00 | 27.57 |
| ATOM | 1052 | CA | ARG | 1622 | 15.056 | 4.776 | 4.066 | 1.00 | 26.47 |
| ATOM | 1053 | CB | ARG | 1622 | 14.233 | 5.918 | 3.460 | 1.00 | 20.08 |
| ATOM | 1054 | CG | ARG | 1622 | 13.762 | 5.634 | 2.077 | 1.00 | 15.87 |
| ATOM | 1055 | CD | ARG | 1622 | 12.998 | 6.791 | 1.501 | 0.50 | 11.86 |
| ATOM | 1056 | NE | ARG | 1622 | 12.613 | 6.458 | 0.144 | 0.50 | 12.46 |
| ATOM | 1057 | CZ | ARG | 1622 | 11.537 | 5.748 | -0.178 | 0.50 | 11.18 |
| ATOM | 1058 | NH1 | ARG | 1622 | 10.711 | 5.304 | 0.767 | 0.50 | 7.16 |
| ATOM | 1059 | NH2 | ARG | 1622 | 11.340 | 5.398 | -1.442 | 0.50 | 9.57 |
| ATOM | 1060 | C | ARG | 1622 | 15.813 | 5.250 | 5.325 | 1.00 | 26.18 |
| ATOM | 1061 | O | ARG | 1622 | 16.645 | 6.150 | 5.250 | 1.00 | 26.90 |
| ATOM | 1062 | N | ASP | 1623 | 15.544 | 4.650 | 6.480 | 1.00 | 27.26 |
| ATOM | 1063 | CA | ASP | 1623 | 16.268 | 5.042 | 7.684 | 1.00 | 29.80 |
| ATOM | 1064 | CB | ASP | 1623 | 15.714 | 6.330 | 8.292 | 1.00 | 32.13 |
| ATOM | 1065 | CG | ASP | 1623 | 16.690 | 6.940 | 9.298 | 1.00 | 37.87 |
| ATOM | 1066 | OD1 | ASP | 1623 | 16.237 | 7.671 | 10.202 | 1.00 | 42.95 |
| ATOM | 1067 | OD2 | ASP | 1623 | 17.907 | 6.684 | 9.191 | 1.00 | 41.09 |
| ATOM | 1068 | C | ASP | 1623 | 16.364 | 3.943 | 8.738 | 1.00 | 29.10 |
| ATOM | 1069 | O | ASP | 1623 | 16.164 | 4.168 | 9.939 | 1.00 | 27.69 |
| ATOM | 1070 | N | LEU | 1624 | 16.723 | 2.755 | 8.270 | 1.00 | 28.23 |
| ATOM | 1071 | CA | LEU | 1624 | 16.874 | 1.599 | 9.129 | 1.00 | 26.00 |
| ATOM | 1072 | CB | LEU | 1624 | 16.944 | 0.351 | 8.245 | 1.00 | 22.14 |
| ATOM | 1073 | CG | LEU | 1624 | 17.036 | -0.998 | 8.941 | 1.00 | 22.32 |
| ATOM | 1074 | CD1 | LEU | 1624 | 15.853 | -1.196 | 9.932 | 1.00 | 17.01 |
| ATOM | 1075 | CD2 | LEU | 1624 | 17.068 | -2.064 | 7.848 | 1.00 | 20.50 |
| ATOM | 1076 | C | LEU | 1624 | 18.129 | 1.757 | 10.003 | 1.00 | 25.89 |
| ATOM | 1077 | O | LEU | 1624 | 19.247 | 1.917 | 9.499 | 1.00 | 26.11 |
| ATOM | 1078 | N | ALA | 1625 | 17.930 | 1.706 | 11.316 | 1.00 | 25.58 |
| ATOM | 1079 | CA | ALA | 1625 | 19.006 | 1.864 | 12.292 | 1.00 | 23.16 |
| ATOM | 1080 | CB | ALA | 1625 | 19.323 | 3.340 | 12.493 | 1.00 | 19.06 |
| ATOM | 1081 | C | ALA | 1625 | 18.475 | 1.286 | 13.584 | 1.00 | 24.12 |
| ATOM | 1082 | O | ALA | 1625 | 17.269 | 1.083 | 13.721 | 1.00 | 27.40 |
| ATOM | 1083 | N | ALA | 1626 | 19.357 | 1.041 | 14.543 | 1.00 | 24.67 |
| ATOM | 1084 | CA | ALA | 1626 | 18.929 | 0.491 | 15.827 | 1.00 | 25.07 |
| ATOM | 1085 | CB | ALA | 1626 | 20.148 | 0.145 | 16.691 | 1.00 | 26.06 |
| ATOM | 1086 | C | ALA | 1626 | 18.015 | 1.474 | 16.560 | 1.00 | 25.13 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1087 | O | ALA | 1626 | 17.184 | 1.069 | 17.366 | 1.00 | 26.38 |
| ATOM | 1088 | N | ARG | 1627 | 18.197 | 2.770 | 16.308 | 1.00 | 23.08 |
| ATOM | 1089 | CA | ARG | 1627 | 17.367 | 3.784 | 16.939 | 1.00 | 24.05 |
| ATOM | 1090 | CB | ARG | 1627 | 17.850 | 5.187 | 16.565 | 1.00 | 28.05 |
| ATOM | 1091 | CG | ARG | 1627 | 17.731 | 5.501 | 15.078 | 1.00 | 37.58 |
| ATOM | 1092 | CD | ARG | 1627 | 18.159 | 6.920 | 14.740 | 1.00 | 42.10 |
| ATOM | 1093 | NE | ARG | 1627 | 18.448 | 7.085 | 13.310 | 1.00 | 42.67 |
| ATOM | 1094 | CZ | ARG | 1627 | 19.667 | 7.006 | 12.784 | 1.00 | 43.58 |
| ATOM | 1095 | NH1 | ARG | 1627 | 20.717 | 6.752 | 13.561 | 1.00 | 46.17 |
| ATOM | 1096 | NH2 | ARG | 1627 | 19.841 | 7.201 | 11.492 | 1.00 | 43.78 |
| ATOM | 1097 | C | ARG | 1627 | 15.926 | 3.632 | 16.482 | 1.00 | 23.04 |
| ATOM | 1098 | O | ARG | 1627 | 15.015 | 3.979 | 17.216 | 1.00 | 22.27 |
| ATOM | 1099 | N | ASN | 1628 | 15.722 | 3.093 | 15.286 | 1.00 | 24.49 |
| ATOM | 1100 | CA | ASN | 1628 | 14.382 | 2.934 | 14.723 | 1.00 | 23.80 |
| ATOM | 1101 | CB | ASN | 1628 | 14.351 | 3.407 | 13.269 | 1.00 | 27.82 |
| ATOM | 1102 | CG | ASN | 1628 | 14.503 | 4.918 | 13.143 | 1.00 | 30.25 |
| ATOM | 1103 | OD1 | ASN | 1628 | 13.876 | 5.686 | 13.863 | 1.00 | 32.33 |
| ATOM | 1104 | ND2 | ASN | 1628 | 15.361 | 5.348 | 12.220 | 1.00 | 31.50 |
| ATOM | 1105 | C | ASN | 1628 | 13.782 | 1.524 | 14.833 | 1.00 | 23.93 |
| ATOM | 1106 | O | ASN | 1628 | 12.896 | 1.161 | 14.056 | 1.00 | 23.64 |
| ATOM | 1107 | N | VAL | 1629 | 14.307 | 0.733 | 15.763 | 1.00 | 24.10 |
| ATOM | 1108 | CA | VAL | 1629 | 13.778 | -0.610 | 16.036 | 1.00 | 22.59 |
| ATOM | 1109 | CB | VAL | 1629 | 14.829 | -1.727 | 15.823 | 1.00 | 21.16 |
| ATOM | 1110 | CG1 | VAL | 1629 | 14.346 | -3.014 | 16.462 | 1.00 | 17.53 |
| ATOM | 1111 | CG2 | VAL | 1629 | 15.068 | -1.962 | 14.341 | 1.00 | 14.48 |
| ATOM | 1112 | C | VAL | 1629 | 13.411 | -0.575 | 17.520 | 1.00 | 24.81 |
| ATOM | 1113 | O | VAL | 1629 | 14.237 | -0.204 | 18.357 | 1.00 | 24.09 |
| ATOM | 1114 | N | LEU | 1630 | 12.181 | -0.941 | 17.850 | 1.00 | 24.34 |
| ATOM | 1115 | CA | LEU | 1630 | 11.751 | -0.919 | 19.239 | 1.00 | 26.53 |
| ATOM | 1116 | CB | LEU | 1630 | 10.447 | -0.129 | 19.359 | 1.00 | 26.19 |
| ATOM | 1117 | CG | LEU | 1630 | 10.522 | 1.293 | 18.758 | 1.00 | 24.33 |
| ATOM | 1118 | CD1 | LEU | 1630 | 9.149 | 1.870 | 18.601 | 1.00 | 20.51 |
| ATOM | 1119 | CD2 | LEU | 1630 | 11.339 | 2.196 | 19.618 | 1.00 | 19.77 |
| ATOM | 1120 | C | LEU | 1630 | 11.641 | -2.327 | 19.835 | 1.00 | 28.14 |
| ATOM | 1121 | O | LEU | 1630 | 11.475 | -3.320 | 19.108 | 1.00 | 28.31 |
| ATOM | 1122 | N | VAL | 1631 | 11.792 | -2.418 | 21.153 | 1.00 | 28.21 |
| ATOM | 1123 | CA | VAL | 1631 | 11.741 | -3.694 | 21.866 | 1.00 | 26.96 |
| ATOM | 1124 | CB | VAL | 1631 | 13.068 | -3.930 | 22.624 | 1.00 | 25.71 |
| ATOM | 1125 | CG1 | VAL | 1631 | 13.113 | -5.345 | 23.222 | 1.00 | 20.40 |
| ATOM | 1126 | CG2 | VAL | 1631 | 14.240 | -3.688 | 21.680 | 1.00 | 19.88 |
| ATOM | 1127 | C | VAL | 1631 | 10.560 | -3.758 | 22.836 | 1.00 | 29.84 |
| ATOM | 1128 | O | VAL | 1631 | 10.419 | -2.918 | 23.738 | 1.00 | 32.46 |
| ATOM | 1129 | N | THR | 1632 | 9.703 | -4.756 | 22.641 | 1.00 | 30.90 |
| ATOM | 1130 | CA | THR | 1632 | 8.530 | -4.939 | 23.487 | 1.00 | 31.16 |
| ATOM | 1131 | CB | THR | 1632 | 7.476 | -5.800 | 22.793 | 1.00 | 29.58 |
| ATOM | 1132 | OG1 | THR | 1632 | 7.948 | -7.152 | 22.708 | 1.00 | 29.17 |
| ATOM | 1133 | CG2 | THR | 1632 | 7.186 | -5.262 | 21.414 | 1.00 | 22.23 |
| ATOM | 1134 | C | THR | 1632 | 8.882 | -5.603 | 24.809 | 1.00 | 32.23 |
| ATOM | 1135 | O | THR | 1632 | 9.950 | -6.185 | 24.946 | 1.00 | 33.23 |
| ATOM | 1136 | N | GLU | 1633 | 7.946 | -5.589 | 25.751 | 1.00 | 34.38 |
| ATOM | 1137 | CA | GLU | 1633 | 8.165 | -6.193 | 27.062 | 1.00 | 35.51 |
| ATOM | 1138 | CB | GLU | 1633 | 6.881 | -6.114 | 27.899 | 1.00 | 35.48 |

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ATOM   1139  CG  GLU  1633       7.004  -6.685  29.309  1.00 45.16
ATOM   1140  CD  GLU  1633       8.070  -5.999  30.183  1.00 50.45
ATOM   1141  OE1 GLU  1633       8.174  -4.750  30.163  1.00 52.70
ATOM   1142  OE2 GLU  1633       8.789  -6.723  30.919  1.00 53.59
ATOM   1143  C   GLU  1633       8.624  -7.635  26.930  1.00 35.40
ATOM   1144  O   GLU  1633       9.387  -8.119  27.758  1.00 36.57
ATOM   1145  N   ASP  1634       8.204  -8.308  25.861  1.00 36.76
ATOM   1146  CA  ASP  1634       8.573  -9.709  25.662  1.00 37.95
ATOM   1147  CB  ASP  1634       7.435 -10.491  24.991  1.00 42.90
ATOM   1148  CG  ASP  1634       6.100 -10.315  25.706  1.00 49.06
ATOM   1149  OD1 ASP  1634       5.885 -10.957  26.759  1.00 50.95
ATOM   1150  OD2 ASP  1634       5.256  -9.544  25.197  1.00 53.92
ATOM   1151  C   ASP  1634       9.842  -9.882  24.840  1.00 36.05
ATOM   1152  O   ASP  1634      10.148 -10.988  24.414  1.00 34.95
ATOM   1153  N   ASN  1635      10.582  -8.787  24.655  1.00 36.53
ATOM   1154  CA  ASN  1635      11.833  -8.763  23.868  1.00 36.21
ATOM   1155  CB  ASN  1635      12.893  -9.692  24.471  1.00 37.91
ATOM   1156  CG  ASN  1635      13.335  -9.244  25.840  1.00 37.60
ATOM   1157  OD1 ASN  1635      13.496  -8.057  26.088  1.00 42.72
ATOM   1158  ND2 ASN  1635      13.525 -10.191  26.743  1.00 38.03
ATOM   1159  C   ASN  1635      11.641  -9.073  22.372  1.00 34.59
ATOM   1160  O   ASN  1635      12.431  -9.799  21.754  1.00 33.52
ATOM   1161  N   VAL  1636      10.557  -8.541  21.819  1.00 31.95
ATOM   1162  CA  VAL  1636      10.260  -8.722  20.415  1.00 28.92
ATOM   1163  CB  VAL  1636       8.743  -8.945  20.177  1.00 31.00
ATOM   1164  CG1 VAL  1636       8.451  -9.066  18.678  1.00 29.52
ATOM   1165  CG2 VAL  1636       8.289 -10.220  20.884  1.00 29.03
ATOM   1166  C   VAL  1636      10.725  -7.461  19.721  1.00 28.05
ATOM   1167  O   VAL  1636      10.432  -6.355  20.179  1.00 25.21
ATOM   1168  N   MET  1637      11.567  -7.637  18.707  1.00 28.78
ATOM   1169  CA  MET  1637      12.107  -6.539  17.927  1.00 27.29
ATOM   1170  CB  MET  1637      13.325  -7.008  17.138  1.00 27.97
ATOM   1171  CG  MET  1637      14.446  -7.576  17.982  1.00 29.31
ATOM   1172  SD  MET  1637      15.051  -6.440  19.245  1.00 29.58
ATOM   1173  CE  MET  1637      15.163  -7.542  20.648  1.00 23.51
ATOM   1174  C   MET  1637      11.033  -6.108  16.951  1.00 26.60
ATOM   1175  O   MET  1637      10.479  -6.951  16.244  1.00 26.60
ATOM   1176  N   LYS  1638      10.758  -4.805  16.893  1.00 24.35
ATOM   1177  CA  LYS  1638       9.745  -4.255  16.006  1.00 20.79
ATOM   1178  CB  LYS  1638       8.495  -3.883  16.793  1.00 18.95
ATOM   1179  CG  LYS  1638       7.723  -5.087  17.268  1.00 22.82
ATOM   1180  CD  LYS  1638       6.442  -4.699  17.969  1.00 25.49
ATOM   1181  CE  LYS  1638       5.560  -5.934  18.189  1.00 24.36
ATOM   1182  NZ  LYS  1638       4.892  -6.414  16.941  1.00 22.23
ATOM   1183  C   LYS  1638      10.254  -3.034  15.257  1.00 22.79
ATOM   1184  O   LYS  1638      10.613  -2.041  15.868  1.00 24.60
ATOM   1185  N   ILE  1639      10.259  -3.101  13.934  1.00 23.92
ATOM   1186  CA  ILE  1639      10.707  -1.984  13.113  1.00 24.22
ATOM   1187  CB  ILE  1639      10.925  -2.439  11.648  1.00 23.18
ATOM   1188  CG2 ILE  1639      11.270  -1.262  10.766  1.00 17.17
ATOM   1189  CG1 ILE  1639      12.068  -3.454  11.604  1.00 19.97
ATOM   1190  CD1 ILE  1639      11.975  -4.369  10.461  1.00 26.92
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1191 | C | ILE | 1639 | 9.686 | -0.846 | 13.173 | 1.00 | 25.63 |
| ATOM | 1192 | O | ILE | 1639 | 8.473 | -1.075 | 13.042 | 1.00 | 26.20 |
| ATOM | 1193 | N | ALA | 1640 | 10.200 | 0.364 | 13.390 | 1.00 | 27.31 |
| ATOM | 1194 | CA | ALA | 1640 | 9.394 | 1.577 | 13.497 | 1.00 | 27.45 |
| ATOM | 1195 | CB | ALA | 1640 | 9.623 | 2.211 | 14.862 | 1.00 | 27.20 |
| ATOM | 1196 | C | ALA | 1640 | 9.720 | 2.595 | 12.411 | 1.00 | 27.87 |
| ATOM | 1197 | O | ALA | 1640 | 10.765 | 2.522 | 11.755 | 1.00 | 26.95 |
| ATOM | 1198 | N | ASP | 1641 | 8.815 | 3.551 | 12.237 | 1.00 | 29.66 |
| ATOM | 1199 | CA | ASP | 1641 | 8.952 | 4.631 | 11.259 | 1.00 | 31.25 |
| ATOM | 1200 | CB | ASP | 1641 | 10.096 | 5.581 | 11.646 | 1.00 | 33.40 |
| ATOM | 1201 | CG | ASP | 1641 | 9.713 | 6.551 | 12.771 | 1.00 | 33.86 |
| ATOM | 1202 | OD1 | ASP | 1641 | 10.475 | 7.524 | 12.953 | 1.00 | 37.57 |
| ATOM | 1203 | OD2 | ASP | 1641 | 8.684 | 6.355 | 13.470 | 1.00 | 29.83 |
| ATOM | 1204 | C | ASP | 1641 | 9.088 | 4.228 | 9.799 | 1.00 | 30.77 |
| ATOM | 1205 | O | ASP | 1641 | 9.526 | 5.022 | 8.966 | 1.00 | 29.52 |
| ATOM | 1206 | N | PHE | 1642 | 8.611 | 3.032 | 9.477 | 1.00 | 30.38 |
| ATOM | 1207 | CA | PHE | 1642 | 8.664 | 2.528 | 8.114 | 1.00 | 29.43 |
| ATOM | 1208 | CB | PHE | 1642 | 8.459 | 1.009 | 8.100 | 1.00 | 25.46 |
| ATOM | 1209 | CG | PHE | 1642 | 7.167 | 0.555 | 8.697 | 1.00 | 20.44 |
| ATOM | 1210 | CD1 | PHE | 1642 | 6.002 | 0.547 | 7.942 | 1.00 | 22.76 |
| ATOM | 1211 | CD2 | PHE | 1642 | 7.119 | 0.112 | 10.007 | 1.00 | 18.52 |
| ATOM | 1212 | CE1 | PHE | 1642 | 4.796 | 0.094 | 8.485 | 1.00 | 25.55 |
| ATOM | 1213 | CE2 | PHE | 1642 | 5.926 | -0.341 | 10.559 | 1.00 | 21.76 |
| ATOM | 1214 | CZ | PHE | 1642 | 4.760 | -0.352 | 9.802 | 1.00 | 24.94 |
| ATOM | 1215 | C | PHE | 1642 | 7.686 | 3.242 | 7.163 | 1.00 | 31.03 |
| ATOM | 1216 | O | PHE | 1642 | 7.946 | 3.330 | 5.975 | 1.00 | 35.19 |
| ATOM | 1217 | N | GLY | 1643 | 6.600 | 3.791 | 7.693 | 1.00 | 30.42 |
| ATOM | 1218 | CA | GLY | 1643 | 5.640 | 4.476 | 6.845 | 1.00 | 28.27 |
| ATOM | 1219 | C | GLY | 1643 | 5.736 | 5.991 | 6.874 | 1.00 | 28.46 |
| ATOM | 1220 | O | GLY | 1643 | 4.896 | 6.707 | 6.332 | 1.00 | 24.29 |
| ATOM | 1221 | N | LEU | 1644 | 6.816 | 6.471 | 7.458 | 1.00 | 31.65 |
| ATOM | 1222 | CA | LEU | 1644 | 7.077 | 7.890 | 7.601 | 1.00 | 36.03 |
| ATOM | 1223 | CB | LEU | 1644 | 8.363 | 8.058 | 8.389 | 1.00 | 32.41 |
| ATOM | 1224 | CG | LEU | 1644 | 8.321 | 9.137 | 9.446 | 1.00 | 35.30 |
| ATOM | 1225 | CD1 | LEU | 1644 | 7.161 | 8.827 | 10.384 | 1.00 | 37.60 |
| ATOM | 1226 | CD2 | LEU | 1644 | 9.663 | 9.186 | 10.190 | 1.00 | 36.62 |
| ATOM | 1227 | C | LEU | 1644 | 7.178 | 8.708 | 6.293 | 1.00 | 40.21 |
| ATOM | 1228 | O | LEU | 1644 | 7.770 | 8.267 | 5.312 | 1.00 | 40.65 |
| ATOM | 1229 | N | ALA | 1645 | 6.553 | 9.881 | 6.293 | 1.00 | 44.50 |
| ATOM | 1230 | CA | ALA | 1645 | 6.591 | 10.786 | 5.148 | 1.00 | 48.66 |
| ATOM | 1231 | CB | ALA | 1645 | 5.432 | 11.762 | 5.241 | 1.00 | 45.63 |
| ATOM | 1232 | C | ALA | 1645 | 7.935 | 11.545 | 5.173 | 1.00 | 51.32 |
| ATOM | 1233 | O | ALA | 1645 | 8.254 | 12.200 | 6.163 | 1.00 | 52.68 |
| ATOM | 1234 | N | ALA | 1646 | 8.727 | 11.444 | 4.107 | 1.00 | 52.77 |
| ATOM | 1235 | CA | ALA | 1646 | 10.023 | 12.121 | 4.077 | 1.00 | 54.73 |
| ATOM | 1236 | CB | ALA | 1646 | 11.108 | 11.194 | 4.646 | 1.00 | 55.34 |
| ATOM | 1237 | C | ALA | 1646 | 10.446 | 12.601 | 2.692 | 1.00 | 56.41 |
| ATOM | 1238 | O | ALA | 1646 | 10.430 | 11.823 | 1.740 | 1.00 | 57.76 |
| ATOM | 1239 | N | ASP | 1647 | 10.811 | 13.876 | 2.567 | 1.00 | 58.20 |
| ATOM | 1240 | CA | ASP | 1647 | 11.280 | 14.394 | 1.283 | 1.00 | 59.39 |
| ATOM | 1241 | CB | ASP | 1647 | 10.898 | 15.861 | 1.083 | 1.00 | 59.29 |
| ATOM | 1242 | CG | ASP | 1647 | 11.128 | 16.339 | -0.356 | 1.00 | 60.67 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1243 | OD1 | ASP | 1647 | 12.110 | 15.908 | -1.009 | 1.00 | 61.21 |
| ATOM | 1244 | OD2 | ASP | 1647 | 10.337 | 17.173 | -0.835 | 1.00 | 61.34 |
| ATOM | 1245 | C | ASP | 1647 | 12.793 | 14.236 | 1.273 | 1.00 | 60.16 |
| ATOM | 1246 | O | ASP | 1647 | 13.523 | 15.023 | 1.889 | 1.00 | 58.16 |
| ATOM | 1247 | N | ILE | 1648 | 13.248 | 13.209 | 0.562 | 1.00 | 61.28 |
| ATOM | 1248 | CA | ILE | 1648 | 14.658 | 12.878 | 0.439 | 1.00 | 62.12 |
| ATOM | 1249 | CB | ILE | 1648 | 14.848 | 11.626 | -0.444 | 1.00 | 59.97 |
| ATOM | 1250 | CG2 | ILE | 1648 | 14.023 | 10.469 | 0.131 | 1.00 | 58.26 |
| ATOM | 1251 | CG1 | ILE | 1648 | 14.429 | 11.922 | -1.883 | 1.00 | 55.69 |
| ATOM | 1252 | CD1 | ILE | 1648 | 15.005 | 10.976 | -2.890 | 1.00 | 54.38 |
| ATOM | 1253 | C | ILE | 1648 | 15.470 | 14.047 | -0.127 | 1.00 | 65.02 |
| ATOM | 1254 | O | ILE | 1648 | 16.633 | 14.245 | 0.233 | 1.00 | 66.85 |
| ATOM | 1255 | N | HIS | 1649 | 14.844 | 14.839 | -0.995 | 1.00 | 65.85 |
| ATOM | 1256 | CA | HIS | 1649 | 15.505 | 15.992 | -1.589 | 1.00 | 66.73 |
| ATOM | 1257 | CB | HIS | 1649 | 14.859 | 16.358 | -2.934 | 1.00 | 65.67 |
| ATOM | 1258 | CG | HIS | 1649 | 15.142 | 15.388 | -4.038 | 1.00 | 66.47 |
| ATOM | 1259 | CD2 | HIS | 1649 | 16.253 | 14.686 | -4.355 | 1.00 | 67.11 |
| ATOM | 1260 | ND1 | HIS | 1649 | 14.210 | 15.064 | -4.999 | 1.00 | 65.21 |
| ATOM | 1261 | CE1 | HIS | 1649 | 14.733 | 14.216 | -5.867 | 1.00 | 66.52 |
| ATOM | 1262 | NE2 | HIS | 1649 | 15.974 | 13.966 | -5.494 | 1.00 | 66.25 |
| ATOM | 1263 | C | HIS | 1649 | 15.505 | 17.200 | -0.663 | 1.00 | 68.55 |
| ATOM | 1264 | O | HIS | 1649 | 15.636 | 18.341 | -1.116 | 1.00 | 69.35 |
| ATOM | 1265 | N | HIS | 1650 | 15.273 | 16.963 | 0.629 | 1.00 | 71.25 |
| ATOM | 1266 | CA | HIS | 1650 | 15.262 | 18.026 | 1.633 | 1.00 | 73.53 |
| ATOM | 1267 | CB | HIS | 1650 | 13.849 | 18.551 | 1.860 | 1.00 | 76.79 |
| ATOM | 1268 | CG | HIS | 1650 | 13.342 | 19.448 | 0.765 | 1.00 | 83.36 |
| ATOM | 1269 | CD2 | HIS | 1650 | 13.509 | 20.772 | 0.537 | 1.00 | 86.47 |
| ATOM | 1270 | ND1 | HIS | 1650 | 12.571 | 18.984 | -0.270 | 1.00 | 87.02 |
| ATOM | 1271 | CE1 | HIS | 1650 | 12.279 | 19.983 | -1.076 | 1.00 | 88.66 |
| ATOM | 1272 | NE2 | HIS | 1650 | 12.840 | 21.080 | -0.609 | 1.00 | 88.34 |
| ATOM | 1273 | C | HIS | 1650 | 15.872 | 17.580 | 2.965 | 1.00 | 73.11 |
| ATOM | 1274 | O | HIS | 1650 | 15.686 | 18.241 | 3.977 | 1.00 | 73.23 |
| ATOM | 1275 | N | ILE | 1651 | 16.599 | 16.464 | 2.949 | 1.00 | 72.64 |
| ATOM | 1276 | CA | ILE | 1651 | 17.234 | 15.937 | 4.143 | 1.00 | 72.54 |
| ATOM | 1277 | CB | ILE | 1651 | 17.660 | 14.472 | 3.942 | 1.00 | 74.59 |
| ATOM | 1278 | CG2 | ILE | 1651 | 18.463 | 13.966 | 5.142 | 1.00 | 75.52 |
| ATOM | 1279 | CG1 | ILE | 1651 | 16.426 | 13.591 | 3.752 | 1.00 | 77.59 |
| ATOM | 1280 | CD1 | ILE | 1651 | 16.747 | 12.141 | 3.472 | 1.00 | 80.12 |
| ATOM | 1281 | C | ILE | 1651 | 18.463 | 16.769 | 4.523 | 1.00 | 71.47 |
| ATOM | 1282 | O | ILE | 1651 | 19.326 | 17.022 | 3.688 | 1.00 | 72.40 |
| ATOM | 1283 | N | ASP | 1652 | 18.529 | 17.197 | 5.784 | 1.00 | 70.34 |
| ATOM | 1284 | CA | ASP | 1652 | 19.678 | 17.976 | 6.235 | 1.00 | 68.57 |
| ATOM | 1285 | CB | ASP | 1652 | 19.272 | 18.878 | 7.411 | 1.00 | 72.80 |
| ATOM | 1286 | CG | ASP | 1652 | 20.456 | 19.640 | 7.982 | 1.00 | 76.90 |
| ATOM | 1287 | OD1 | ASP | 1652 | 21.463 | 19.888 | 7.287 | 1.00 | 79.62 |
| ATOM | 1288 | OD2 | ASP | 1652 | 20.369 | 20.030 | 9.170 | 1.00 | 80.36 |
| ATOM | 1289 | C | ASP | 1652 | 20.771 | 17.007 | 6.652 | 1.00 | 66.01 |
| ATOM | 1290 | O | ASP | 1652 | 20.709 | 16.421 | 7.735 | 1.00 | 64.75 |
| ATOM | 1291 | N | TYR | 1653 | 21.778 | 16.868 | 5.808 | 1.00 | 64.05 |
| ATOM | 1292 | CA | TYR | 1653 | 22.906 | 15.978 | 6.074 | 1.00 | 63.55 |
| ATOM | 1293 | CB | TYR | 1653 | 23.829 | 15.913 | 4.855 | 1.00 | 63.81 |
| ATOM | 1294 | CG | TYR | 1653 | 23.316 | 14.993 | 3.771 | 1.00 | 65.65 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1295 | CD1 | TYR | 1653 | 24.082 | 14.710 | 2.643 | 1.00 | 65.32 |
| ATOM | 1296 | CE1 | TYR | 1653 | 23.638 | 13.810 | 1.674 | 1.00 | 68.40 |
| ATOM | 1297 | CD2 | TYR | 1653 | 22.079 | 14.357 | 3.903 | 1.00 | 66.72 |
| ATOM | 1298 | CE2 | TYR | 1653 | 21.626 | 13.451 | 2.940 | 1.00 | 69.93 |
| ATOM | 1299 | CZ | TYR | 1653 | 22.409 | 13.182 | 1.833 | 1.00 | 70.13 |
| ATOM | 1300 | OH | TYR | 1653 | 21.966 | 12.272 | 0.902 | 1.00 | 72.73 |
| ATOM | 1301 | C | TYR | 1653 | 23.708 | 16.334 | 7.328 | 1.00 | 62.96 |
| ATOM | 1302 | O | TYR | 1653 | 24.342 | 15.473 | 7.938 | 1.00 | 63.31 |
| ATOM | 1303 | N | TYR | 1654 | 23.653 | 17.598 | 7.727 | 1.00 | 63.02 |
| ATOM | 1304 | CA | TYR | 1654 | 24.379 | 18.065 | 8.902 | 1.00 | 63.89 |
| ATOM | 1305 | CB | TYR | 1654 | 24.896 | 19.491 | 8.684 | 1.00 | 60.37 |
| ATOM | 1306 | CG | TYR | 1654 | 26.012 | 19.565 | 7.669 | 1.00 | 59.33 |
| ATOM | 1307 | CD1 | TYR | 1654 | 25.735 | 19.673 | 6.313 | 1.00 | 59.29 |
| ATOM | 1308 | CE1 | TYR | 1654 | 26.759 | 19.687 | 5.362 | 1.00 | 61.50 |
| ATOM | 1309 | CD2 | TYR | 1654 | 27.349 | 19.480 | 8.061 | 1.00 | 60.05 |
| ATOM | 1310 | CE2 | TYR | 1654 | 28.384 | 19.498 | 7.119 | 1.00 | 61.35 |
| ATOM | 1311 | CZ | TYR | 1654 | 28.082 | 19.598 | 5.773 | 1.00 | 62.41 |
| ATOM | 1312 | OH | TYR | 1654 | 29.098 | 19.589 | 4.842 | 1.00 | 60.57 |
| ATOM | 1313 | C | TYR | 1654 | 23.586 | 17.984 | 10.192 | 1.00 | 65.65 |
| ATOM | 1314 | O | TYR | 1654 | 24.104 | 18.321 | 11.252 | 1.00 | 67.31 |
| ATOM | 1315 | N | LYS | 1655 | 22.349 | 17.504 | 10.118 | 1.00 | 67.52 |
| ATOM | 1316 | CA | LYS | 1655 | 21.499 | 17.390 | 11.303 | 1.00 | 69.54 |
| ATOM | 1317 | CB | LYS | 1655 | 20.028 | 17.445 | 10.893 | 1.00 | 71.09 |
| ATOM | 1318 | CG | LYS | 1655 | 19.057 | 17.518 | 12.049 | 1.00 | 73.08 |
| ATOM | 1319 | CD | LYS | 1655 | 17.648 | 17.713 | 11.531 | 1.00 | 76.73 |
| ATOM | 1320 | CE | LYS | 1655 | 16.624 | 17.320 | 12.568 | 1.00 | 81.94 |
| ATOM | 1321 | NZ | LYS | 1655 | 15.232 | 17.521 | 12.072 | 1.00 | 84.53 |
| ATOM | 1322 | C | LYS | 1655 | 21.783 | 16.102 | 12.076 | 1.00 | 70.33 |
| ATOM | 1323 | O | LYS | 1655 | 21.952 | 15.032 | 11.478 | 1.00 | 70.43 |
| ATOM | 1324 | N | LYS | 1656 | 21.825 | 16.218 | 13.403 | 1.00 | 70.11 |
| ATOM | 1325 | CA | LYS | 1656 | 22.093 | 15.079 | 14.274 | 1.00 | 70.03 |
| ATOM | 1326 | CB | LYS | 1656 | 23.049 | 15.481 | 15.394 | 1.00 | 67.72 |
| ATOM | 1327 | CG | LYS | 1656 | 24.473 | 15.716 | 14.947 | 1.00 | 66.34 |
| ATOM | 1328 | CD | LYS | 1656 | 25.326 | 16.124 | 16.136 | 1.00 | 66.60 |
| ATOM | 1329 | CE | LYS | 1656 | 26.801 | 15.839 | 15.905 | 1.00 | 64.71 |
| ATOM | 1330 | NZ | LYS | 1656 | 27.612 | 16.059 | 17.138 | 1.00 | 62.24 |
| ATOM | 1331 | C | LYS | 1656 | 20.823 | 14.480 | 14.881 | 1.00 | 70.67 |
| ATOM | 1332 | O | LYS | 1656 | 19.759 | 15.104 | 14.864 | 1.00 | 71.91 |
| ATOM | 1333 | N | THR | 1657 | 20.941 | 13.265 | 15.412 | 1.00 | 69.38 |
| ATOM | 1334 | CA | THR | 1657 | 19.818 | 12.586 | 16.035 | 1.00 | 68.30 |
| ATOM | 1335 | CB | THR | 1657 | 20.052 | 11.051 | 16.101 | 1.00 | 69.30 |
| ATOM | 1336 | OG1 | THR | 1657 | 21.179 | 10.757 | 16.941 | 1.00 | 68.20 |
| ATOM | 1337 | CG2 | THR | 1657 | 20.310 | 10.479 | 14.713 | 1.00 | 69.71 |
| ATOM | 1338 | C | THR | 1657 | 19.706 | 13.145 | 17.445 | 1.00 | 67.60 |
| ATOM | 1339 | O | THR | 1657 | 20.521 | 13.971 | 17.846 | 1.00 | 67.40 |
| ATOM | 1340 | N | ALA | 1658 | 18.715 | 12.694 | 18.206 | 1.00 | 67.83 |
| ATOM | 1341 | CA | ALA | 1658 | 18.564 | 13.163 | 19.582 | 1.00 | 67.73 |
| ATOM | 1342 | CB | ALA | 1658 | 17.345 | 12.503 | 20.234 | 1.00 | 68.87 |
| ATOM | 1343 | C | ALA | 1658 | 19.833 | 12.820 | 20.364 | 1.00 | 66.59 |
| ATOM | 1344 | O | ALA | 1658 | 20.368 | 13.640 | 21.115 | 1.00 | 66.33 |
| ATOM | 1345 | N | ASN | 1659 | 20.343 | 11.616 | 20.129 | 1.00 | 65.38 |
| ATOM | 1346 | CA | ASN | 1659 | 21.545 | 11.143 | 20.801 | 1.00 | 62.65 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1347 | CB | ASN | 1659 | 21.702 | 9.638 | 20.616 | 1.00 | 63.61 |
| ATOM | 1348 | CG | ASN | 1659 | 22.548 | 9.009 | 21.697 | 1.00 | 64.09 |
| ATOM | 1349 | OD1 | ASN | 1659 | 22.526 | 9.451 | 22.850 | 1.00 | 63.69 |
| ATOM | 1350 | ND2 | ASN | 1659 | 23.279 | 7.959 | 21.345 | 1.00 | 64.10 |
| ATOM | 1351 | C | ASN | 1659 | 22.808 | 11.844 | 20.321 | 1.00 | 60.46 |
| ATOM | 1352 | O | ASN | 1659 | 23.882 | 11.601 | 20.856 | 1.00 | 60.78 |
| ATOM | 1353 | N | GLY | 1660 | 22.671 | 12.675 | 19.285 | 1.00 | 58.84 |
| ATOM | 1354 | CA | GLY | 1660 | 23.803 | 13.407 | 18.735 | 1.00 | 56.69 |
| ATOM | 1355 | C | GLY | 1660 | 24.570 | 12.721 | 17.616 | 1.00 | 56.40 |
| ATOM | 1356 | O | GLY | 1660 | 25.738 | 13.028 | 17.377 | 1.00 | 56.43 |
| ATOM | 1357 | N | ARG | 1661 | 23.929 | 11.779 | 16.937 | 1.00 | 56.00 |
| ATOM | 1358 | CA | ARG | 1661 | 24.585 | 11.048 | 15.849 | 1.00 | 53.80 |
| ATOM | 1359 | CB | ARG | 1661 | 24.312 | 9.540 | 15.952 | 1.00 | 54.52 |
| ATOM | 1360 | CG | ARG | 1661 | 24.876 | 8.879 | 17.218 | 1.00 | 55.28 |
| ATOM | 1361 | CD | ARG | 1661 | 24.556 | 7.395 | 17.226 | 1.00 | 58.01 |
| ATOM | 1362 | NE | ARG | 1661 | 25.051 | 6.670 | 18.396 | 1.00 | 58.41 |
| ATOM | 1363 | CZ | ARG | 1661 | 24.918 | 5.355 | 18.559 | 1.00 | 59.08 |
| ATOM | 1364 | NH1 | ARG | 1661 | 24.306 | 4.637 | 17.623 | 1.00 | 55.82 |
| ATOM | 1365 | NH2 | ARG | 1661 | 25.394 | 4.762 | 19.652 | 1.00 | 57.53 |
| ATOM | 1366 | C | ARG | 1661 | 24.139 | 11.581 | 14.491 | 1.00 | 51.03 |
| ATOM | 1367 | O | ARG | 1661 | 23.160 | 12.323 | 14.401 | 1.00 | 48.69 |
| ATOM | 1368 | N | LEU | 1662 | 24.859 | 11.189 | 13.440 | 1.00 | 48.33 |
| ATOM | 1369 | CA | LEU | 1662 | 24.565 | 11.647 | 12.087 | 1.00 | 45.87 |
| ATOM | 1370 | CB | LEU | 1662 | 25.839 | 12.199 | 11.426 | 1.00 | 46.18 |
| ATOM | 1371 | CG | LEU | 1662 | 26.374 | 13.511 | 12.016 | 1.00 | 45.78 |
| ATOM | 1372 | CD1 | LEU | 1662 | 27.856 | 13.681 | 11.722 | 1.00 | 45.92 |
| ATOM | 1373 | CD2 | LEU | 1662 | 25.576 | 14.698 | 11.489 | 1.00 | 44.92 |
| ATOM | 1374 | C | LEU | 1662 | 23.961 | 10.542 | 11.230 | 1.00 | 43.02 |
| ATOM | 1375 | O | LEU | 1662 | 24.647 | 9.607 | 10.811 | 1.00 | 42.04 |
| ATOM | 1376 | N | PRO | 1663 | 22.648 | 10.640 | 10.968 | 1.00 | 41.48 |
| ATOM | 1377 | CD | PRO | 1663 | 21.769 | 11.718 | 11.468 | 1.00 | 40.54 |
| ATOM | 1378 | CA | PRO | 1663 | 21.886 | 9.680 | 10.161 | 1.00 | 39.60 |
| ATOM | 1379 | CB | PRO | 1663 | 20.582 | 10.424 | 9.889 | 1.00 | 38.77 |
| ATOM | 1380 | CG | PRO | 1663 | 20.386 | 11.183 | 11.151 | 1.00 | 40.83 |
| ATOM | 1381 | C | PRO | 1663 | 22.578 | 9.273 | 8.860 | 1.00 | 35.90 |
| ATOM | 1382 | O | PRO | 1663 | 22.448 | 8.124 | 8.427 | 1.00 | 36.85 |
| ATOM | 1383 | N | VAL | 1664 | 23.356 | 10.180 | 8.276 | 1.00 | 33.16 |
| ATOM | 1384 | CA | VAL | 1664 | 24.053 | 9.880 | 7.024 | 1.00 | 32.51 |
| ATOM | 1385 | CB | VAL | 1664 | 24.851 | 11.106 | 6.439 | 1.00 | 32.44 |
| ATOM | 1386 | CG1 | VAL | 1664 | 23.917 | 12.213 | 6.065 | 1.00 | 26.99 |
| ATOM | 1387 | CG2 | VAL | 1664 | 25.897 | 11.607 | 7.421 | 1.00 | 29.84 |
| ATOM | 1388 | C | VAL | 1664 | 24.989 | 8.675 | 7.158 | 1.00 | 30.30 |
| ATOM | 1389 | O | VAL | 1664 | 25.400 | 8.091 | 6.161 | 1.00 | 30.16 |
| ATOM | 1390 | N | LYS | 1665 | 25.278 | 8.276 | 8.393 | 1.00 | 27.72 |
| ATOM | 1391 | CA | LYS | 1665 | 26.170 | 7.151 | 8.649 | 1.00 | 27.96 |
| ATOM | 1392 | CB | LYS | 1665 | 26.808 | 7.276 | 10.025 | 1.00 | 26.42 |
| ATOM | 1393 | CG | LYS | 1665 | 27.857 | 8.351 | 10.061 | 1.00 | 28.20 |
| ATOM | 1394 | CD | LYS | 1665 | 28.221 | 8.754 | 11.478 | 1.00 | 32.47 |
| ATOM | 1395 | CE | LYS | 1665 | 29.398 | 9.720 | 11.468 | 1.00 | 32.33 |
| ATOM | 1396 | NZ | LYS | 1665 | 29.713 | 10.231 | 12.819 | 1.00 | 30.38 |
| ATOM | 1397 | C | LYS | 1665 | 25.522 | 5.794 | 8.486 | 1.00 | 25.81 |
| ATOM | 1398 | O | LYS | 1665 | 26.159 | 4.769 | 8.691 | 1.00 | 27.53 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1399 | N | TRP | 1666 | 24.247 | 5.793 | 8.120 | 1.00 | 26.13 |
| ATOM | 1400 | CA | TRP | 1666 | 23.499 | 4.554 | 7.896 | 1.00 | 25.88 |
| ATOM | 1401 | CB | TRP | 1666 | 22.259 | 4.537 | 8.800 | 1.00 | 26.15 |
| ATOM | 1402 | CG | TRP | 1666 | 22.547 | 4.067 | 10.226 | 1.00 | 28.12 |
| ATOM | 1403 | CD2 | TRP | 1666 | 23.020 | 4.864 | 11.324 | 1.00 | 26.14 |
| ATOM | 1404 | CE2 | TRP | 1666 | 23.154 | 4.009 | 12.438 | 1.00 | 24.97 |
| ATOM | 1405 | CE3 | TRP | 1666 | 23.349 | 6.225 | 11.475 | 1.00 | 25.14 |
| ATOM | 1406 | CD1 | TRP | 1666 | 22.408 | 2.795 | 10.715 | 1.00 | 26.09 |
| ATOM | 1407 | NE1 | TRP | 1666 | 22.777 | 2.751 | 12.034 | 1.00 | 22.55 |
| ATOM | 1408 | CZ2 | TRP | 1666 | 23.606 | 4.453 | 13.684 | 1.00 | 25.32 |
| ATOM | 1409 | CZ3 | TRP | 1666 | 23.795 | 6.664 | 12.712 | 1.00 | 21.72 |
| ATOM | 1410 | CH2 | TRP | 1666 | 23.920 | 5.782 | 13.798 | 1.00 | 23.77 |
| ATOM | 1411 | C | TRP | 1666 | 23.092 | 4.444 | 6.425 | 1.00 | 24.79 |
| ATOM | 1412 | O | TRP | 1666 | 22.662 | 3.390 | 5.971 | 1.00 | 25.26 |
| ATOM | 1413 | N | MET | 1667 | 23.350 | 5.508 | 5.664 | 1.00 | 24.21 |
| ATOM | 1414 | CA | MET | 1667 | 22.963 | 5.568 | 4.252 | 1.00 | 23.79 |
| ATOM | 1415 | CB | MET | 1667 | 22.796 | 7.018 | 3.809 | 1.00 | 25.08 |
| ATOM | 1416 | CG | MET | 1667 | 21.793 | 7.813 | 4.564 | 1.00 | 32.58 |
| ATOM | 1417 | SD | MET | 1667 | 21.778 | 9.495 | 3.910 | 1.00 | 41.43 |
| ATOM | 1418 | CE | MET | 1667 | 21.011 | 9.209 | 2.387 | 1.00 | 40.85 |
| ATOM | 1419 | C | MET | 1667 | 23.938 | 4.942 | 3.279 | 1.00 | 22.52 |
| ATOM | 1420 | O | MET | 1667 | 25.139 | 5.173 | 3.362 | 1.00 | 23.63 |
| ATOM | 1421 | N | ALA | 1668 | 23.406 | 4.195 | 2.324 | 1.00 | 22.77 |
| ATOM | 1422 | CA | ALA | 1668 | 24.218 | 3.576 | 1.278 | 1.00 | 24.91 |
| ATOM | 1423 | CB | ALA | 1668 | 23.342 | 2.672 | 0.396 | 1.00 | 24.41 |
| ATOM | 1424 | C | ALA | 1668 | 24.800 | 4.706 | 0.438 | 1.00 | 26.66 |
| ATOM | 1425 | O | ALA | 1668 | 24.163 | 5.748 | 0.251 | 1.00 | 24.54 |
| ATOM | 1426 | N | PRO | 1669 | 26.011 | 4.511 | -0.101 | 1.00 | 26.97 |
| ATOM | 1427 | CD | PRO | 1669 | 26.935 | 3.374 | 0.066 | 1.00 | 26.23 |
| ATOM | 1428 | CA | PRO | 1669 | 26.614 | 5.563 | -0.919 | 1.00 | 26.05 |
| ATOM | 1429 | CB | PRO | 1669 | 27.855 | 4.876 | -1.482 | 1.00 | 24.03 |
| ATOM | 1430 | CG | PRO | 1669 | 28.259 | 3.946 | -0.358 | 1.00 | 26.27 |
| ATOM | 1431 | C | PRO | 1669 | 25.687 | 6.048 | -2.030 | 1.00 | 26.44 |
| ATOM | 1432 | O | PRO | 1669 | 25.576 | 7.250 | -2.263 | 1.00 | 27.72 |
| ATOM | 1433 | N | GLU | 1670 | 24.971 | 5.137 | -2.685 | 1.00 | 27.16 |
| ATOM | 1434 | CA | GLU | 1670 | 24.093 | 5.553 | -3.769 | 1.00 | 27.63 |
| ATOM | 1435 | CB | GLU | 1670 | 23.613 | 4.365 | -4.614 | 1.00 | 29.35 |
| ATOM | 1436 | CG | GLU | 1670 | 22.545 | 3.492 | -3.980 | 1.00 | 29.16 |
| ATOM | 1437 | CD | GLU | 1670 | 23.089 | 2.238 | -3.310 | 1.00 | 28.03 |
| ATOM | 1438 | OE1 | GLU | 1670 | 22.248 | 1.430 | -2.874 | 1.00 | 24.12 |
| ATOM | 1439 | OE2 | GLU | 1670 | 24.325 | 2.040 | -3.215 | 1.00 | 26.07 |
| ATOM | 1440 | C | GLU | 1670 | 22.931 | 6.407 | -3.301 | 1.00 | 25.52 |
| ATOM | 1441 | O | GLU | 1670 | 22.477 | 7.281 | -4.042 | 1.00 | 24.12 |
| ATOM | 1442 | N | ALA | 1671 | 22.452 | 6.163 | -2.084 | 1.00 | 27.74 |
| ATOM | 1443 | CA | ALA | 1671 | 21.337 | 6.928 | -1.510 | 1.00 | 27.65 |
| ATOM | 1444 | CB | ALA | 1671 | 20.729 | 6.189 | -0.319 | 1.00 | 23.18 |
| ATOM | 1445 | C | ALA | 1671 | 21.860 | 8.283 | -1.065 | 1.00 | 28.22 |
| ATOM | 1446 | O | ALA | 1671 | 21.234 | 9.310 | -1.305 | 1.00 | 28.51 |
| ATOM | 1447 | N | LEU | 1672 | 23.011 | 8.266 | -0.406 | 1.00 | 30.60 |
| ATOM | 1448 | CA | LEU | 1672 | 23.647 | 9.484 | 0.074 | 1.00 | 32.67 |
| ATOM | 1449 | CB | LEU | 1672 | 24.831 | 9.127 | 0.952 | 1.00 | 32.05 |
| ATOM | 1450 | CG | LEU | 1672 | 25.662 | 10.264 | 1.527 | 1.00 | 34.00 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1451 | CD1 | LEU | 1672 | 24.874 | 10.981 | 2.577 | 1.00 | 38.85 |
| ATOM | 1452 | CD2 | LEU | 1672 | 26.910 | 9.667 | 2.149 | 1.00 | 35.22 |
| ATOM | 1453 | C | LEU | 1672 | 24.121 | 10.398 | -1.067 | 1.00 | 37.10 |
| ATOM | 1454 | O | LEU | 1672 | 23.799 | 11.580 | -1.086 | 1.00 | 37.19 |
| ATOM | 1455 | N | PHE | 1673 | 24.905 | 9.858 | -1.997 | 1.00 | 37.60 |
| ATOM | 1456 | CA | PHE | 1673 | 25.403 | 10.664 | -3.102 | 1.00 | 37.11 |
| ATOM | 1457 | CB | PHE | 1673 | 26.692 | 10.061 | -3.667 | 1.00 | 35.24 |
| ATOM | 1458 | CG | PHE | 1673 | 27.782 | 9.857 | -2.644 | 1.00 | 33.54 |
| ATOM | 1459 | CD1 | PHE | 1673 | 28.456 | 8.633 | -2.566 | 1.00 | 31.54 |
| ATOM | 1460 | CD2 | PHE | 1673 | 28.143 | 10.874 | -1.762 | 1.00 | 33.10 |
| ATOM | 1461 | CE1 | PHE | 1673 | 29.467 | 8.421 | -1.623 | 1.00 | 34.66 |
| ATOM | 1462 | CE2 | PHE | 1673 | 29.156 | 10.678 | -0.816 | 1.00 | 35.41 |
| ATOM | 1463 | CZ | PHE | 1673 | 29.819 | 9.444 | -0.748 | 1.00 | 34.81 |
| ATOM | 1464 | C | PHE | 1673 | 24.406 | 10.890 | -4.245 | 1.00 | 39.03 |
| ATOM | 1465 | O | PHE | 1673 | 24.276 | 11.997 | -4.734 | 1.00 | 39.02 |
| ATOM | 1466 | N | ASP | 1674 | 23.693 | 9.844 | -4.651 | 1.00 | 42.35 |
| ATOM | 1467 | CA | ASP | 1674 | 22.757 | 9.931 | -5.762 | 1.00 | 41.59 |
| ATOM | 1468 | CB | ASP | 1674 | 22.957 | 8.736 | -6.700 | 1.00 | 46.08 |
| ATOM | 1469 | CG | ASP | 1674 | 24.384 | 8.617 | -7.201 | 1.00 | 51.20 |
| ATOM | 1470 | OD1 | ASP | 1674 | 25.057 | 9.663 | -7.333 | 1.00 | 53.97 |
| ATOM | 1471 | OD2 | ASP | 1674 | 24.822 | 7.470 | -7.469 | 1.00 | 50.65 |
| ATOM | 1472 | C | ASP | 1674 | 21.263 | 9.999 | -5.418 | 1.00 | 42.89 |
| ATOM | 1473 | O | ASP | 1674 | 20.427 | 10.079 | -6.317 | 1.00 | 41.95 |
| ATOM | 1474 | N | ARG | 1675 | 20.923 | 9.899 | -4.134 | 1.00 | 42.82 |
| ATOM | 1475 | CA | ARG | 1675 | 19.521 | 9.944 | -3.706 | 1.00 | 42.64 |
| ATOM | 1476 | CB | ARG | 1675 | 18.890 | 11.300 | -4.028 | 1.00 | 48.80 |
| ATOM | 1477 | CG | ARG | 1675 | 19.480 | 12.449 | -3.252 | 1.00 | 61.19 |
| ATOM | 1478 | CD | ARG | 1675 | 19.407 | 13.727 | -4.068 | 1.00 | 72.90 |
| ATOM | 1479 | NE | ARG | 1675 | 20.025 | 14.854 | -3.381 | 1.00 | 83.15 |
| ATOM | 1480 | CZ | ARG | 1675 | 19.652 | 16.123 | -3.539 | 1.00 | 88.21 |
| ATOM | 1481 | NH1 | ARG | 1675 | 18.662 | 16.439 | -4.365 | 1.00 | 89.58 |
| ATOM | 1482 | NH2 | ARG | 1675 | 20.265 | 17.085 | -2.860 | 1.00 | 92.07 |
| ATOM | 1483 | C | ARG | 1675 | 18.674 | 8.825 | -4.299 | 1.00 | 38.05 |
| ATOM | 1484 | O | ARG | 1675 | 17.495 | 9.005 | -4.588 | 1.00 | 38.87 |
| ATOM | 1485 | N | ILE | 1676 | 19.281 | 7.658 | -4.479 | 1.00 | 34.44 |
| ATOM | 1486 | CA | ILE | 1676 | 18.576 | 6.514 | -5.012 | 1.00 | 30.11 |
| ATOM | 1487 | CB | ILE | 1676 | 19.378 | 5.825 | -6.096 | 1.00 | 29.58 |
| ATOM | 1488 | CG2 | ILE | 1676 | 18.509 | 4.850 | -6.797 | 1.00 | 30.72 |
| ATOM | 1489 | CG1 | ILE | 1676 | 19.835 | 6.868 | -7.116 | 1.00 | 34.29 |
| ATOM | 1490 | CD1 | ILE | 1676 | 20.798 | 6.348 | -8.145 | 1.00 | 41.15 |
| ATOM | 1491 | C | ILE | 1676 | 18.315 | 5.541 | -3.874 | 1.00 | 26.90 |
| ATOM | 1492 | O | ILE | 1676 | 19.236 | 4.898 | -3.364 | 1.00 | 22.06 |
| ATOM | 1493 | N | TYR | 1677 | 17.056 | 5.465 | -3.454 | 1.00 | 28.17 |
| ATOM | 1494 | CA | TYR | 1677 | 16.677 | 4.589 | -2.350 | 1.00 | 26.80 |
| ATOM | 1495 | CB | TYR | 1677 | 15.742 | 5.310 | -1.398 | 1.00 | 26.05 |
| ATOM | 1496 | CG | TYR | 1677 | 16.442 | 6.367 | -0.580 | 1.00 | 26.92 |
| ATOM | 1497 | CD1 | TYR | 1677 | 16.510 | 7.693 | -1.018 | 1.00 | 23.98 |
| ATOM | 1498 | CE1 | TYR | 1677 | 17.129 | 8.665 | -0.250 | 1.00 | 23.90 |
| ATOM | 1499 | CD2 | TYR | 1677 | 17.022 | 6.048 | 0.644 | 1.00 | 26.99 |
| ATOM | 1500 | CE2 | TYR | 1677 | 17.642 | 7.017 | 1.414 | 1.00 | 24.87 |
| ATOM | 1501 | CZ | TYR | 1677 | 17.685 | 8.315 | 0.968 | 1.00 | 26.44 |
| ATOM | 1502 | OH | TYR | 1677 | 18.227 | 9.273 | 1.783 | 1.00 | 30.89 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1503 | C | TYR | 1677 | 16.006 | 3.350 | -2.894 | 1.00 | 26.30 |
| ATOM | 1504 | O | TYR | 1677 | 15.080 | 3.445 | -3.703 | 1.00 | 28.12 |
| ATOM | 1505 | N | THR | 1678 | 16.489 | 2.197 | -2.458 | 1.00 | 25.46 |
| ATOM | 1506 | CA | THR | 1678 | 15.973 | 0.918 | -2.927 | 1.00 | 26.27 |
| ATOM | 1507 | CB | THR | 1678 | 16.904 | 0.336 | -3.994 | 1.00 | 28.43 |
| ATOM | 1508 | OG1 | THR | 1678 | 18.185 | 0.095 | -3.405 | 1.00 | 30.59 |
| ATOM | 1509 | CG2 | THR | 1678 | 17.068 | 1.305 | -5.174 | 1.00 | 26.56 |
| ATOM | 1510 | C | THR | 1678 | 15.987 | -0.049 | -1.758 | 1.00 | 24.60 |
| ATOM | 1511 | O | THR | 1678 | 16.476 | 0.277 | -0.693 | 1.00 | 27.15 |
| ATOM | 1512 | N | HIS | 1679 | 15.500 | -1.260 | -1.974 | 1.00 | 23.23 |
| ATOM | 1513 | CA | HIS | 1679 | 15.496 | -2.276 | -0.933 | 1.00 | 21.51 |
| ATOM | 1514 | CB | HIS | 1679 | 14.747 | -3.520 | -1.411 | 1.00 | 20.84 |
| ATOM | 1515 | CG | HIS | 1679 | 13.297 | -3.279 | -1.695 | 1.00 | 21.48 |
| ATOM | 1516 | CD2 | HIS | 1679 | 12.552 | -3.476 | -2.812 | 1.00 | 22.71 |
| ATOM | 1517 | ND1 | HIS | 1679 | 12.423 | -2.795 | -0.741 | 1.00 | 27.21 |
| ATOM | 1518 | CE1 | HIS | 1679 | 11.206 | -2.713 | -1.255 | 1.00 | 22.60 |
| ATOM | 1519 | NE2 | HIS | 1679 | 11.255 | -3.116 | -2.515 | 1.00 | 23.66 |
| ATOM | 1520 | C | HIS | 1679 | 16.976 | -2.591 | -0.665 | 1.00 | 20.81 |
| ATOM | 1521 | O | HIS | 1679 | 17.358 | -2.954 | 0.451 | 1.00 | 22.50 |
| ATOM | 1522 | N | GLN | 1680 | 17.799 | -2.382 | -1.695 | 1.00 | 19.58 |
| ATOM | 1523 | CA | GLN | 1680 | 19.248 | -2.587 | -1.657 | 1.00 | 20.89 |
| ATOM | 1524 | CB | GLN | 1680 | 19.860 | -2.400 | -3.038 | 1.00 | 23.76 |
| ATOM | 1525 | CG | GLN | 1680 | 19.896 | -3.651 | -3.877 | 1.00 | 34.08 |
| ATOM | 1526 | CD | GLN | 1680 | 19.015 | -3.559 | -5.096 | 1.00 | 37.77 |
| ATOM | 1527 | OE1 | GLN | 1680 | 18.069 | -2.780 | -5.122 | 1.00 | 43.23 |
| ATOM | 1528 | NE2 | GLN | 1680 | 19.321 | -4.356 | -6.113 | 1.00 | 37.02 |
| ATOM | 1529 | C | GLN | 1680 | 19.913 | -1.609 | -0.724 | 1.00 | 20.72 |
| ATOM | 1530 | O | GLN | 1680 | 20.814 | -1.981 | 0.021 | 1.00 | 21.53 |
| ATOM | 1531 | N | SER | 1681 | 19.514 | -0.350 | -0.773 | 1.00 | 21.01 |
| ATOM | 1532 | CA | SER | 1681 | 20.128 | 0.606 | 0.135 | 1.00 | 23.86 |
| ATOM | 1533 | CB | SER | 1681 | 19.841 | 2.065 | -0.248 | 1.00 | 21.10 |
| ATOM | 1534 | OG | SER | 1681 | 18.473 | 2.290 | -0.506 | 1.00 | 23.18 |
| ATOM | 1535 | C | SER | 1681 | 19.695 | 0.292 | 1.564 | 1.00 | 23.91 |
| ATOM | 1536 | O | SER | 1681 | 20.457 | 0.542 | 2.495 | 1.00 | 26.70 |
| ATOM | 1537 | N | ASP | 1682 | 18.511 | -0.303 | 1.739 | 1.00 | 21.71 |
| ATOM | 1538 | CA | ASP | 1682 | 18.044 | -0.662 | 3.080 | 1.00 | 21.28 |
| ATOM | 1539 | CB | ASP | 1682 | 16.595 | -1.149 | 3.070 | 1.00 | 23.22 |
| ATOM | 1540 | CG | ASP | 1682 | 15.569 | -0.016 | 3.198 | 1.00 | 23.08 |
| ATOM | 1541 | OD1 | ASP | 1682 | 14.363 | -0.282 | 3.017 | 1.00 | 21.99 |
| ATOM | 1542 | OD2 | ASP | 1682 | 15.948 | 1.135 | 3.498 | 1.00 | 24.42 |
| ATOM | 1543 | C | ASP | 1682 | 18.955 | -1.756 | 3.611 | 1.00 | 20.86 |
| ATOM | 1544 | O | ASP | 1682 | 19.289 | -1.770 | 4.799 | 1.00 | 21.62 |
| ATOM | 1545 | N | VAL | 1683 | 19.398 | -2.649 | 2.727 | 1.00 | 21.60 |
| ATOM | 1546 | CA | VAL | 1683 | 20.307 | -3.732 | 3.122 | 1.00 | 22.27 |
| ATOM | 1547 | CB | VAL | 1683 | 20.515 | -4.740 | 1.965 | 1.00 | 22.22 |
| ATOM | 1548 | CG1 | VAL | 1683 | 21.587 | -5.777 | 2.315 | 1.00 | 21.52 |
| ATOM | 1549 | CG2 | VAL | 1683 | 19.187 | -5.437 | 1.662 | 1.00 | 20.89 |
| ATOM | 1550 | C | VAL | 1683 | 21.618 | -3.150 | 3.666 | 1.00 | 21.96 |
| ATOM | 1551 | O | VAL | 1683 | 22.107 | -3.577 | 4.705 | 1.00 | 24.39 |
| ATOM | 1552 | N | TRP | 1684 | 22.172 | -2.160 | 2.970 | 1.00 | 22.01 |
| ATOM | 1553 | CA | TRP | 1684 | 23.375 | -1.489 | 3.449 | 1.00 | 23.06 |
| ATOM | 1554 | CB | TRP | 1684 | 23.685 | -0.273 | 2.566 | 1.00 | 20.25 |

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| ATOM | 1555 | CG | TRP | 1684 | 24.808 | 0.549 | 3.069 | 1.00 | 22.35 |
| ATOM | 1556 | CD2 | TRP | 1684 | 26.118 | 0.644 | 2.503 | 1.00 | 24.14 |
| ATOM | 1557 | CE2 | TRP | 1684 | 26.879 | 1.500 | 3.334 | 1.00 | 23.68 |
| ATOM | 1558 | CE3 | TRP | 1684 | 26.728 | 0.091 | 1.370 | 1.00 | 25.09 |
| ATOM | 1559 | CD1 | TRP | 1684 | 24.825 | 1.346 | 4.193 | 1.00 | 22.52 |
| ATOM | 1560 | NE1 | TRP | 1684 | 26.066 | 1.915 | 4.355 | 1.00 | 21.48 |
| ATOM | 1561 | CZ2 | TRP | 1684 | 28.216 | 1.815 | 3.061 | 1.00 | 20.56 |
| ATOM | 1562 | CZ3 | TRP | 1684 | 28.059 | 0.405 | 1.095 | 1.00 | 23.92 |
| ATOM | 1563 | CH2 | TRP | 1684 | 28.785 | 1.257 | 1.942 | 1.00 | 23.18 |
| ATOM | 1564 | C | TRP | 1684 | 23.105 | -1.025 | 4.903 | 1.00 | 23.96 |
| ATOM | 1565 | O | TRP | 1684 | 23.889 | -1.308 | 5.815 | 1.00 | 25.98 |
| ATOM | 1566 | N | SER | 1685 | 21.992 | -0.332 | 5.118 | 1.00 | 24.68 |
| ATOM | 1567 | CA | SER | 1685 | 21.615 | 0.144 | 6.447 | 1.00 | 22.75 |
| ATOM | 1568 | CB | SER | 1685 | 20.266 | 0.870 | 6.376 | 1.00 | 21.11 |
| ATOM | 1569 | OG | SER | 1685 | 20.276 | 1.950 | 5.452 | 1.00 | 21.98 |
| ATOM | 1570 | C | SER | 1685 | 21.516 | -1.011 | 7.457 | 1.00 | 23.06 |
| ATOM | 1571 | O | SER | 1685 | 21.865 | -0.850 | 8.638 | 1.00 | 22.55 |
| ATOM | 1572 | N | PHE | 1686 | 21.041 | -2.168 | 6.998 | 1.00 | 21.83 |
| ATOM | 1573 | CA | PHE | 1686 | 20.915 | -3.340 | 7.854 | 1.00 | 21.92 |
| ATOM | 1574 | CB | PHE | 1686 | 20.153 | -4.457 | 7.129 | 1.00 | 18.02 |
| ATOM | 1575 | CG | PHE | 1686 | 19.965 | -5.683 | 7.971 | 1.00 | 20.86 |
| ATOM | 1576 | CD1 | PHE | 1686 | 19.142 | -5.641 | 9.108 | 1.00 | 18.76 |
| ATOM | 1577 | CD2 | PHE | 1686 | 20.669 | -6.853 | 7.688 | 1.00 | 18.96 |
| ATOM | 1578 | CE1 | PHE | 1686 | 19.023 | -6.743 | 9.947 | 1.00 | 19.29 |
| ATOM | 1579 | CE2 | PHE | 1686 | 20.554 | -7.965 | 8.514 | 1.00 | 19.27 |
| ATOM | 1580 | CZ | PHE | 1686 | 19.732 | -7.908 | 9.653 | 1.00 | 21.91 |
| ATOM | 1581 | C | PHE | 1686 | 22.304 | -3.845 | 8.316 | 1.00 | 22.11 |
| ATOM | 1582 | O | PHE | 1686 | 22.473 | -4.378 | 9.436 | 1.00 | 21.35 |
| ATOM | 1583 | N | GLY | 1687 | 23.294 | -3.691 | 7.436 | 1.00 | 20.48 |
| ATOM | 1584 | CA | GLY | 1687 | 24.653 | -4.079 | 7.769 | 1.00 | 20.41 |
| ATOM | 1585 | C | GLY | 1687 | 25.185 | -3.211 | 8.899 | 1.00 | 19.03 |
| ATOM | 1586 | O | GLY | 1687 | 25.857 | -3.714 | 9.808 | 1.00 | 20.27 |
| ATOM | 1587 | N | VAL | 1688 | 24.893 | -1.906 | 8.829 | 1.00 | 20.57 |
| ATOM | 1588 | CA | VAL | 1688 | 25.296 | -0.937 | 9.860 | 1.00 | 21.14 |
| ATOM | 1589 | CB | VAL | 1688 | 24.974 | 0.548 | 9.467 | 1.00 | 20.78 |
| ATOM | 1590 | CG1 | VAL | 1688 | 25.440 | 1.493 | 10.564 | 1.00 | 21.51 |
| ATOM | 1591 | CG2 | VAL | 1688 | 25.681 | 0.923 | 8.186 | 1.00 | 19.70 |
| ATOM | 1592 | C | VAL | 1688 | 24.547 | -1.297 | 11.142 | 1.00 | 23.16 |
| ATOM | 1593 | O | VAL | 1688 | 25.126 | -1.271 | 12.225 | 1.00 | 24.14 |
| ATOM | 1594 | N | LEU | 1689 | 23.264 | -1.648 | 11.021 | 1.00 | 24.50 |
| ATOM | 1595 | CA | LEU | 1689 | 22.465 | -2.058 | 12.187 | 1.00 | 25.93 |
| ATOM | 1596 | CB | LEU | 1689 | 21.008 | -2.316 | 11.776 | 1.00 | 25.42 |
| ATOM | 1597 | CG | LEU | 1689 | 19.933 | -2.392 | 12.874 | 1.00 | 26.29 |
| ATOM | 1598 | CD1 | LEU | 1689 | 18.572 | -2.053 | 12.272 | 1.00 | 23.43 |
| ATOM | 1599 | CD2 | LEU | 1689 | 19.885 | -3.768 | 13.543 | 1.00 | 25.66 |
| ATOM | 1600 | C | LEU | 1689 | 23.080 | -3.330 | 12.797 | 1.00 | 28.01 |
| ATOM | 1601 | O | LEU | 1689 | 23.203 | -3.426 | 14.016 | 1.00 | 30.06 |
| ATOM | 1602 | N | LEU | 1690 | 23.487 | -4.287 | 11.956 | 1.00 | 27.19 |
| ATOM | 1603 | CA | LEU | 1690 | 24.111 | -5.520 | 12.457 | 1.00 | 25.29 |
| ATOM | 1604 | CB | LEU | 1690 | 24.556 | -6.446 | 11.315 | 1.00 | 24.98 |
| ATOM | 1605 | CG | LEU | 1690 | 23.594 | -7.390 | 10.589 | 1.00 | 24.85 |
| ATOM | 1606 | CD1 | LEU | 1690 | 24.385 | -8.132 | 9.538 | 1.00 | 24.22 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1607 | CD2 | LEU | 1690 | 22.960 | -8.434 | 11.512 | 1.00 | 19.10 |
| ATOM | 1608 | C | LEU | 1690 | 25.326 | -5.123 | 13.291 | 1.00 | 24.70 |
| ATOM | 1609 | O | LEU | 1690 | 25.521 | -5.624 | 14.408 | 1.00 | 23.57 |
| ATOM | 1610 | N | TRP | 1691 | 26.117 | -4.197 | 12.747 | 1.00 | 23.68 |
| ATOM | 1611 | CA | TRP | 1691 | 27.316 | -3.693 | 13.425 | 1.00 | 24.83 |
| ATOM | 1612 | CB | TRP | 1691 | 27.998 | -2.621 | 12.567 | 1.00 | 20.94 |
| ATOM | 1613 | CG | TRP | 1691 | 29.331 | -2.173 | 13.105 | 1.00 | 24.80 |
| ATOM | 1614 | CD2 | TRP | 1691 | 29.565 | -1.082 | 14.004 | 1.00 | 23.71 |
| ATOM | 1615 | CE2 | TRP | 1691 | 30.966 | -0.996 | 14.208 | 1.00 | 23.81 |
| ATOM | 1616 | CE3 | TRP | 1691 | 28.726 | -0.167 | 14.652 | 1.00 | 22.20 |
| ATOM | 1617 | CD1 | TRP | 1691 | 30.570 | -2.702 | 12.811 | 1.00 | 24.44 |
| ATOM | 1618 | NE1 | TRP | 1691 | 31.550 | -1.995 | 13.471 | 1.00 | 25.38 |
| ATOM | 1619 | CZ2 | TRP | 1691 | 31.543 | -0.022 | 15.034 | 1.00 | 24.39 |
| ATOM | 1620 | CZ3 | TRP | 1691 | 29.300 | 0.799 | 15.484 | 1.00 | 21.99 |
| ATOM | 1621 | CH2 | TRP | 1691 | 30.700 | 0.862 | 15.665 | 1.00 | 25.57 |
| ATOM | 1622 | C | TRP | 1691 | 26.998 | -3.131 | 14.823 | 1.00 | 25.87 |
| ATOM | 1623 | O | TRP | 1691 | 27.772 | -3.301 | 15.750 | 1.00 | 27.39 |
| ATOM | 1624 | N | GLU | 1692 | 25.865 | -2.448 | 14.956 | 1.00 | 26.45 |
| ATOM | 1625 | CA | GLU | 1692 | 25.452 | -1.869 | 16.238 | 1.00 | 25.13 |
| ATOM | 1626 | CB | GLU | 1692 | 24.257 | -0.933 | 16.068 | 1.00 | 23.56 |
| ATOM | 1627 | CG | GLU | 1692 | 24.365 | 0.091 | 14.962 | 1.00 | 18.73 |
| ATOM | 1628 | CD | GLU | 1692 | 23.111 | 0.935 | 14.880 | 1.00 | 23.79 |
| ATOM | 1629 | OE1 | GLU | 1692 | 22.303 | 0.722 | 13.962 | 1.00 | 22.70 |
| ATOM | 1630 | OE2 | GLU | 1692 | 22.919 | 1.819 | 15.738 | 1.00 | 25.63 |
| ATOM | 1631 | C | GLU | 1692 | 25.072 | -2.963 | 17.225 | 1.00 | 25.28 |
| ATOM | 1632 | O | GLU | 1692 | 25.278 | -2.818 | 18.422 | 1.00 | 27.65 |
| ATOM | 1633 | N | ILE | 1693 | 24.484 | -4.046 | 16.720 | 1.00 | 26.23 |
| ATOM | 1634 | CA | ILE | 1693 | 24.080 | -5.164 | 17.565 | 1.00 | 23.81 |
| ATOM | 1635 | CB | ILE | 1693 | 23.177 | -6.203 | 16.787 | 1.00 | 22.99 |
| ATOM | 1636 | CG2 | ILE | 1693 | 22.966 | -7.465 | 17.637 | 1.00 | 21.67 |
| ATOM | 1637 | CG1 | ILE | 1693 | 21.820 | -5.569 | 16.416 | 1.00 | 20.23 |
| ATOM | 1638 | CD1 | ILE | 1693 | 20.964 | -6.395 | 15.435 | 1.00 | 13.67 |
| ATOM | 1639 | C | ILE | 1693 | 25.322 | -5.843 | 18.133 | 1.00 | 24.77 |
| ATOM | 1640 | O | ILE | 1693 | 25.401 | -6.126 | 19.324 | 1.00 | 24.94 |
| ATOM | 1641 | N | PHE | 1694 | 26.329 | -6.051 | 17.304 | 1.00 | 27.59 |
| ATOM | 1642 | CA | PHE | 1694 | 27.503 | -6.709 | 17.827 | 1.00 | 29.42 |
| ATOM | 1643 | CB | PHE | 1694 | 28.122 | -7.623 | 16.771 | 1.00 | 29.37 |
| ATOM | 1644 | CG | PHE | 1694 | 27.142 | -8.649 | 16.263 | 1.00 | 27.99 |
| ATOM | 1645 | CD1 | PHE | 1694 | 26.522 | -8.486 | 15.034 | 1.00 | 28.43 |
| ATOM | 1646 | CD2 | PHE | 1694 | 26.751 | -9.709 | 17.074 | 1.00 | 27.86 |
| ATOM | 1647 | CE1 | PHE | 1694 | 25.525 | -9.355 | 14.625 | 1.00 | 30.12 |
| ATOM | 1648 | CE2 | PHE | 1694 | 25.751 | -10.586 | 16.674 | 1.00 | 25.78 |
| ATOM | 1649 | CZ | PHE | 1694 | 25.136 | -10.408 | 15.453 | 1.00 | 26.17 |
| ATOM | 1650 | C | PHE | 1694 | 28.495 | -5.821 | 18.578 | 1.00 | 29.83 |
| ATOM | 1651 | O | PHE | 1694 | 29.485 | -6.305 | 19.126 | 1.00 | 32.81 |
| ATOM | 1652 | N | THR | 1695 | 28.217 | -4.516 | 18.635 | 1.00 | 28.35 |
| ATOM | 1653 | CA | THR | 1695 | 29.044 | -3.598 | 19.419 | 1.00 | 25.39 |
| ATOM | 1654 | CB | THR | 1695 | 29.540 | -2.379 | 18.627 | 1.00 | 21.81 |
| ATOM | 1655 | OG1 | THR | 1695 | 28.422 | -1.628 | 18.137 | 1.00 | 21.54 |
| ATOM | 1656 | CG2 | THR | 1695 | 30.457 | -2.816 | 17.508 | 1.00 | 16.93 |
| ATOM | 1657 | C | THR | 1695 | 28.198 | -3.126 | 20.604 | 1.00 | 26.16 |
| ATOM | 1658 | O | THR | 1695 | 28.620 | -2.268 | 21.386 | 1.00 | 26.77 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1659 | N | LEU | 1696 | 27.023 | -3.747 | 20.747 | 1.00 | 26.87 |
| ATOM | 1660 | CA | LEU | 1696 | 26.069 | -3.446 | 21.813 | 1.00 | 27.64 |
| ATOM | 1661 | CB | LEU | 1696 | 26.572 | -3.977 | 23.156 | 1.00 | 30.54 |
| ATOM | 1662 | CG | LEU | 1696 | 26.903 | -5.456 | 23.182 | 1.00 | 29.75 |
| ATOM | 1663 | CD1 | LEU | 1696 | 27.448 | -5.821 | 24.546 | 1.00 | 32.53 |
| ATOM | 1664 | CD2 | LEU | 1696 | 25.658 | -6.234 | 22.882 | 1.00 | 33.79 |
| ATOM | 1665 | C | LEU | 1696 | 25.727 | -1.984 | 21.946 | 1.00 | 25.51 |
| ATOM | 1666 | O | LEU | 1696 | 25.824 | -1.410 | 23.025 | 1.00 | 27.90 |
| ATOM | 1667 | N | GLY | 1697 | 25.265 | -1.395 | 20.857 | 1.00 | 26.48 |
| ATOM | 1668 | CA | GLY | 1697 | 24.899 | 0.007 | 20.859 | 1.00 | 25.81 |
| ATOM | 1669 | C | GLY | 1697 | 26.040 | 0.900 | 20.452 | 1.00 | 26.40 |
| ATOM | 1670 | O | GLY | 1697 | 26.055 | 2.090 | 20.760 | 1.00 | 29.69 |
| ATOM | 1671 | N | GLY | 1698 | 27.008 | 0.330 | 19.748 | 1.00 | 27.65 |
| ATOM | 1672 | CA | GLY | 1698 | 28.150 | 1.110 | 19.314 | 1.00 | 28.38 |
| ATOM | 1673 | C | GLY | 1698 | 27.795 | 2.186 | 18.310 | 1.00 | 30.13 |
| ATOM | 1674 | O | GLY | 1698 | 26.896 | 2.028 | 17.496 | 1.00 | 32.55 |
| ATOM | 1675 | N | SER | 1699 | 28.520 | 3.295 | 18.375 | 1.00 | 30.56 |
| ATOM | 1676 | CA | SER | 1699 | 28.304 | 4.420 | 17.491 | 1.00 | 32.11 |
| ATOM | 1677 | CB | SER | 1699 | 28.622 | 5.714 | 18.246 | 1.00 | 33.58 |
| ATOM | 1678 | OG | SER | 1699 | 28.578 | 6.863 | 17.407 | 1.00 | 38.87 |
| ATOM | 1679 | C | SER | 1699 | 29.203 | 4.269 | 16.268 | 1.00 | 32.10 |
| ATOM | 1680 | O | SER | 1699 | 30.408 | 4.073 | 16.403 | 1.00 | 31.12 |
| ATOM | 1681 | N | PRO | 1700 | 28.629 | 4.324 | 15.062 | 1.00 | 32.70 |
| ATOM | 1682 | CD | PRO | 1700 | 27.204 | 4.482 | 14.745 | 1.00 | 34.35 |
| ATOM | 1683 | CA | PRO | 1700 | 29.427 | 4.192 | 13.837 | 1.00 | 32.25 |
| ATOM | 1684 | CB | PRO | 1700 | 28.358 | 4.096 | 12.736 | 1.00 | 32.85 |
| ATOM | 1685 | CG | PRO | 1700 | 27.101 | 3.713 | 13.461 | 1.00 | 35.54 |
| ATOM | 1686 | C | PRO | 1700 | 30.258 | 5.456 | 13.651 | 1.00 | 31.84 |
| ATOM | 1687 | O | PRO | 1700 | 29.792 | 6.550 | 13.983 | 1.00 | 31.56 |
| ATOM | 1688 | N | TYR | 1701 | 31.487 | 5.306 | 13.170 | 1.00 | 31.07 |
| ATOM | 1689 | CA | TYR | 1701 | 32.372 | 6.441 | 12.910 | 1.00 | 32.41 |
| ATOM | 1690 | CB | TYR | 1701 | 32.039 | 7.055 | 11.537 | 1.00 | 32.39 |
| ATOM | 1691 | CG | TYR | 1701 | 32.088 | 6.092 | 10.378 | 1.00 | 35.63 |
| ATOM | 1692 | CD1 | TYR | 1701 | 30.936 | 5.807 | 9.638 | 1.00 | 37.94 |
| ATOM | 1693 | CE1 | TYR | 1701 | 30.977 | 4.955 | 8.535 | 1.00 | 40.79 |
| ATOM | 1694 | CD2 | TYR | 1701 | 33.293 | 5.495 | 9.990 | 1.00 | 37.49 |
| ATOM | 1695 | CE2 | TYR | 1701 | 33.351 | 4.646 | 8.886 | 1.00 | 41.82 |
| ATOM | 1696 | CZ | TYR | 1701 | 32.190 | 4.382 | 8.160 | 1.00 | 45.96 |
| ATOM | 1697 | OH | TYR | 1701 | 32.251 | 3.572 | 7.039 | 1.00 | 55.61 |
| ATOM | 1698 | C | TYR | 1701 | 32.377 | 7.559 | 13.970 | 1.00 | 32.85 |
| ATOM | 1699 | O | TYR | 1701 | 32.066 | 8.711 | 13.679 | 1.00 | 32.41 |
| ATOM | 1700 | N | PRO | 1702 | 32.753 | 7.229 | 15.215 | 1.00 | 34.48 |
| ATOM | 1701 | CD | PRO | 1702 | 33.288 | 5.946 | 15.695 | 1.00 | 35.64 |
| ATOM | 1702 | CA | PRO | 1702 | 32.775 | 8.258 | 16.270 | 1.00 | 33.68 |
| ATOM | 1703 | CB | PRO | 1702 | 33.321 | 7.499 | 17.482 | 1.00 | 32.52 |
| ATOM | 1704 | CG | PRO | 1702 | 33.063 | 6.061 | 17.166 | 1.00 | 38.81 |
| ATOM | 1705 | C | PRO | 1702 | 33.736 | 9.388 | 15.919 | 1.00 | 33.47 |
| ATOM | 1706 | O | PRO | 1702 | 34.875 | 9.145 | 15.522 | 1.00 | 34.66 |
| ATOM | 1707 | N | GLY | 1703 | 33.275 | 10.625 | 16.089 | 1.00 | 35.31 |
| ATOM | 1708 | CA | GLY | 1703 | 34.101 | 11.792 | 15.802 | 1.00 | 32.51 |
| ATOM | 1709 | C | GLY | 1703 | 34.232 | 12.166 | 14.339 | 1.00 | 33.68 |
| ATOM | 1710 | O | GLY | 1703 | 34.904 | 13.146 | 14.005 | 1.00 | 31.22 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1711 | N | VAL | 1704 | 33.583 | 11.404 | 13.462 | 1.00 | 35.00 |
| ATOM | 1712 | CA | VAL | 1704 | 33.641 | 11.658 | 12.026 | 1.00 | 33.25 |
| ATOM | 1713 | CB | VAL | 1704 | 33.679 | 10.335 | 11.241 | 1.00 | 31.04 |
| ATOM | 1714 | CG1 | VAL | 1704 | 33.825 | 10.605 | 9.766 | 1.00 | 32.72 |
| ATOM | 1715 | CG2 | VAL | 1704 | 34.825 | 9.477 | 11.727 | 1.00 | 26.97 |
| ATOM | 1716 | C | VAL | 1704 | 32.475 | 12.529 | 11.533 | 1.00 | 34.75 |
| ATOM | 1717 | O | VAL | 1704 | 31.316 | 12.151 | 11.643 | 1.00 | 36.79 |
| ATOM | 1718 | N | PRO | 1705 | 32.787 | 13.735 | 11.032 | 1.00 | 35.01 |
| ATOM | 1719 | CD | PRO | 1705 | 34.133 | 14.333 | 11.086 | 1.00 | 35.61 |
| ATOM | 1720 | CA | PRO | 1705 | 31.801 | 14.685 | 10.512 | 1.00 | 35.33 |
| ATOM | 1721 | CB | PRO | 1705 | 32.539 | 16.020 | 10.617 | 1.00 | 35.59 |
| ATOM | 1722 | CG | PRO | 1705 | 33.950 | 15.625 | 10.339 | 1.00 | 37.23 |
| ATOM | 1723 | C | PRO | 1705 | 31.388 | 14.375 | 9.074 | 1.00 | 36.33 |
| ATOM | 1724 | O | PRO | 1705 | 32.125 | 13.695 | 8.355 | 1.00 | 38.44 |
| ATOM | 1725 | N | VAL | 1706 | 30.240 | 14.912 | 8.649 | 1.00 | 34.93 |
| ATOM | 1726 | CA | VAL | 1706 | 29.675 | 14.704 | 7.303 | 1.00 | 35.19 |
| ATOM | 1727 | CB | VAL | 1706 | 28.607 | 15.791 | 6.984 | 1.00 | 36.19 |
| ATOM | 1728 | CG1 | VAL | 1706 | 28.011 | 15.586 | 5.586 | 1.00 | 36.30 |
| ATOM | 1729 | CG2 | VAL | 1706 | 27.494 | 15.739 | 8.028 | 1.00 | 32.74 |
| ATOM | 1730 | C | VAL | 1706 | 30.696 | 14.632 | 6.155 | 1.00 | 36.20 |
| ATOM | 1731 | O | VAL | 1706 | 30.796 | 13.618 | 5.463 | 1.00 | 38.16 |
| ATOM | 1732 | N | GLU | 1707 | 31.479 | 15.695 | 6.020 | 1.00 | 34.38 |
| ATOM | 1733 | CA | GLU | 1707 | 32.500 | 15.819 | 4.987 | 1.00 | 33.75 |
| ATOM | 1734 | CB | GLU | 1707 | 33.181 | 17.184 | 5.083 | 1.00 | 35.79 |
| ATOM | 1735 | C | GLU | 1707 | 33.567 | 14.731 | 4.982 | 1.00 | 31.97 |
| ATOM | 1736 | O | GLU | 1707 | 34.036 | 14.311 | 3.923 | 1.00 | 32.84 |
| ATOM | 1737 | N | GLU | 1708 | 33.964 | 14.280 | 6.160 | 1.00 | 29.57 |
| ATOM | 1738 | CA | GLU | 1708 | 34.987 | 13.249 | 6.249 | 1.00 | 31.32 |
| ATOM | 1739 | CB | GLU | 1708 | 35.567 | 13.204 | 7.664 | 1.00 | 36.11 |
| ATOM | 1740 | CG | GLU | 1708 | 36.189 | 14.508 | 8.144 | 1.00 | 44.10 |
| ATOM | 1741 | CD | GLU | 1708 | 37.444 | 14.923 | 7.383 | 1.00 | 55.58 |
| ATOM | 1742 | OE1 | GLU | 1708 | 38.059 | 14.082 | 6.681 | 1.00 | 61.47 |
| ATOM | 1743 | OE2 | GLU | 1708 | 37.830 | 16.115 | 7.517 | 1.00 | 60.54 |
| ATOM | 1744 | C | GLU | 1708 | 34.365 | 11.906 | 5.889 | 1.00 | 32.20 |
| ATOM | 1745 | O | GLU | 1708 | 35.013 | 11.041 | 5.294 | 1.00 | 32.39 |
| ATOM | 1746 | N | LEU | 1709 | 33.094 | 11.749 | 6.245 | 1.00 | 31.43 |
| ATOM | 1747 | CA | LEU | 1709 | 32.378 | 10.522 | 5.961 | 1.00 | 31.71 |
| ATOM | 1748 | CB | LEU | 1709 | 30.973 | 10.548 | 6.565 | 1.00 | 28.84 |
| ATOM | 1749 | CG | LEU | 1709 | 30.136 | 9.357 | 6.081 | 1.00 | 28.28 |
| ATOM | 1750 | CD1 | LEU | 1709 | 30.662 | 8.059 | 6.679 | 1.00 | 27.34 |
| ATOM | 1751 | CD2 | LEU | 1709 | 28.705 | 9.556 | 6.437 | 1.00 | 29.71 |
| ATOM | 1752 | C | LEU | 1709 | 32.306 | 10.317 | 4.454 | 1.00 | 30.55 |
| ATOM | 1753 | O | LEU | 1709 | 32.489 | 9.202 | 3.970 | 1.00 | 31.79 |
| ATOM | 1754 | N | PHE | 1710 | 32.043 | 11.399 | 3.727 | 1.00 | 30.99 |
| ATOM | 1755 | CA | PHE | 1710 | 31.945 | 11.366 | 2.279 | 1.00 | 32.80 |
| ATOM | 1756 | CB | PHE | 1710 | 31.680 | 12.768 | 1.737 | 1.00 | 34.22 |
| ATOM | 1757 | CG | PHE | 1710 | 30.310 | 13.261 | 2.020 | 1.00 | 37.65 |
| ATOM | 1758 | CD1 | PHE | 1710 | 29.337 | 12.393 | 2.495 | 1.00 | 43.43 |
| ATOM | 1759 | CD2 | PHE | 1710 | 29.984 | 14.596 | 1.838 | 1.00 | 42.87 |
| ATOM | 1760 | CE1 | PHE | 1710 | 28.054 | 12.834 | 2.787 | 1.00 | 46.00 |
| ATOM | 1761 | CE2 | PHE | 1710 | 28.698 | 15.053 | 2.130 | 1.00 | 46.30 |
| ATOM | 1762 | CZ | PHE | 1710 | 27.733 | 14.169 | 2.605 | 1.00 | 46.49 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1763 | C | PHE | 1710 | 33.196 | 10.802 | 1.667 | 1.00 | 34.25 |
| ATOM | 1764 | O | PHE | 1710 | 33.133 | 9.948 | 0.785 | 1.00 | 36.09 |
| ATOM | 1765 | N | LYS | 1711 | 34.324 | 11.249 | 2.209 | 1.00 | 34.37 |
| ATOM | 1766 | CA | LYS | 1711 | 35.664 | 10.840 | 1.789 | 1.00 | 34.11 |
| ATOM | 1767 | CB | LYS | 1711 | 36.672 | 11.768 | 2.476 | 1.00 | 37.74 |
| ATOM | 1768 | CG | LYS | 1711 | 38.114 | 11.567 | 2.119 | 1.00 | 43.59 |
| ATOM | 1769 | CD | LYS | 1711 | 38.978 | 12.573 | 2.857 | 1.00 | 46.97 |
| ATOM | 1770 | CE | LYS | 1711 | 40.386 | 12.575 | 2.304 | 1.00 | 51.53 |
| ATOM | 1771 | NZ | LYS | 1711 | 41.074 | 11.291 | 2.603 | 1.00 | 58.84 |
| ATOM | 1772 | C | LYS | 1711 | 35.948 | 9.354 | 2.103 | 1.00 | 33.25 |
| ATOM | 1773 | O | LYS | 1711 | 36.512 | 8.641 | 1.274 | 1.00 | 32.22 |
| ATOM | 1774 | N | LEU | 1712 | 35.537 | 8.894 | 3.285 | 1.00 | 32.62 |
| ATOM | 1775 | CA | LEU | 1712 | 35.718 | 7.496 | 3.667 | 1.00 | 31.41 |
| ATOM | 1776 | CB | LEU | 1712 | 35.223 | 7.237 | 5.106 | 1.00 | 29.80 |
| ATOM | 1777 | CG | LEU | 1712 | 36.020 | 7.889 | 6.244 | 1.00 | 29.22 |
| ATOM | 1778 | CD1 | LEU | 1712 | 35.385 | 7.643 | 7.608 | 1.00 | 24.09 |
| ATOM | 1779 | CD2 | LEU | 1712 | 37.437 | 7.356 | 6.234 | 1.00 | 28.36 |
| ATOM | 1780 | C | LEU | 1712 | 34.939 | 6.638 | 2.674 | 1.00 | 31.88 |
| ATOM | 1781 | O | LEU | 1712 | 35.452 | 5.654 | 2.143 | 1.00 | 34.08 |
| ATOM | 1782 | N | LEU | 1713 | 33.700 | 7.029 | 2.413 | 1.00 | 32.28 |
| ATOM | 1783 | CA | LEU | 1713 | 32.850 | 6.305 | 1.482 | 1.00 | 35.36 |
| ATOM | 1784 | CB | LEU | 1713 | 31.433 | 6.887 | 1.485 | 1.00 | 38.97 |
| ATOM | 1785 | CG | LEU | 1713 | 30.629 | 6.494 | 2.730 | 1.00 | 39.56 |
| ATOM | 1786 | CD1 | LEU | 1713 | 29.308 | 7.228 | 2.768 | 1.00 | 37.14 |
| ATOM | 1787 | CD2 | LEU | 1713 | 30.424 | 4.988 | 2.748 | 1.00 | 37.73 |
| ATOM | 1788 | C | LEU | 1713 | 33.430 | 6.296 | 0.070 | 1.00 | 36.47 |
| ATOM | 1789 | O | LEU | 1713 | 33.502 | 5.244 | -0.563 | 1.00 | 39.32 |
| ATOM | 1790 | N | LYS | 1714 | 33.855 | 7.455 | -0.413 | 1.00 | 35.21 |
| ATOM | 1791 | CA | LYS | 1714 | 34.437 | 7.544 | -1.743 | 1.00 | 34.55 |
| ATOM | 1792 | CB | LYS | 1714 | 34.812 | 8.984 | -2.075 | 1.00 | 34.81 |
| ATOM | 1793 | CG | LYS | 1714 | 33.624 | 9.903 | -2.290 | 1.00 | 36.55 |
| ATOM | 1794 | CD | LYS | 1714 | 32.681 | 9.372 | -3.353 | 1.00 | 40.68 |
| ATOM | 1795 | CE | LYS | 1714 | 31.488 | 10.310 | -3.577 | 1.00 | 44.87 |
| ATOM | 1796 | NZ | LYS | 1714 | 30.611 | 9.853 | -4.701 | 1.00 | 50.99 |
| ATOM | 1797 | C | LYS | 1714 | 35.671 | 6.649 | -1.856 | 1.00 | 35.97 |
| ATOM | 1798 | O | LYS | 1714 | 35.948 | 6.084 | -2.920 | 1.00 | 38.11 |
| ATOM | 1799 | N | GLU | 1715 | 36.385 | 6.490 | -0.749 | 1.00 | 33.65 |
| ATOM | 1800 | CA | GLU | 1715 | 37.582 | 5.663 | -0.729 | 1.00 | 34.34 |
| ATOM | 1801 | CB | GLU | 1715 | 38.574 | 6.221 | 0.288 | 1.00 | 34.90 |
| ATOM | 1802 | CG | GLU | 1715 | 39.032 | 7.613 | -0.110 | 1.00 | 42.07 |
| ATOM | 1803 | CD | GLU | 1715 | 39.729 | 8.405 | 0.989 | 1.00 | 47.94 |
| ATOM | 1804 | OE1 | GLU | 1715 | 39.977 | 7.870 | 2.098 | 1.00 | 45.03 |
| ATOM | 1805 | OE2 | GLU | 1715 | 40.026 | 9.596 | 0.709 | 1.00 | 51.48 |
| ATOM | 1806 | C | GLU | 1715 | 37.285 | 4.191 | -0.466 | 1.00 | 34.76 |
| ATOM | 1807 | O | GLU | 1715 | 38.205 | 3.384 | -0.411 | 1.00 | 37.36 |
| ATOM | 1808 | N | GLY | 1716 | 36.002 | 3.848 | -0.347 | 1.00 | 32.00 |
| ATOM | 1809 | CA | GLY | 1716 | 35.604 | 2.474 | -0.122 | 1.00 | 30.49 |
| ATOM | 1810 | C | GLY | 1716 | 35.932 | 1.937 | 1.251 | 1.00 | 31.32 |
| ATOM | 1811 | O | GLY | 1716 | 36.134 | 0.738 | 1.430 | 1.00 | 31.83 |
| ATOM | 1812 | N | HIS | 1717 | 35.957 | 2.822 | 2.233 | 1.00 | 31.55 |
| ATOM | 1813 | CA | HIS | 1717 | 36.265 | 2.416 | 3.595 | 1.00 | 33.20 |
| ATOM | 1814 | CB | HIS | 1717 | 36.494 | 3.661 | 4.452 | 1.00 | 37.67 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1815 | CG | HIS | 1717 | 36.786 | 3.360 | 5.895 | 1.00 | 42.42 |
| ATOM | 1816 | CD2 | HIS | 1717 | 37.957 | 3.259 | 6.567 | 1.00 | 40.97 |
| ATOM | 1817 | ND1 | HIS | 1717 | 35.789 | 3.142 | 6.825 | 1.00 | 45.02 |
| ATOM | 1818 | CE1 | HIS | 1717 | 36.333 | 2.914 | 8.004 | 1.00 | 44.06 |
| ATOM | 1819 | NE2 | HIS | 1717 | 37.645 | 2.976 | 7.873 | 1.00 | 43.67 |
| ATOM | 1820 | C | HIS | 1717 | 35.149 | 1.567 | 4.201 | 1.00 | 31.72 |
| ATOM | 1821 | O | HIS | 1717 | 33.975 | 1.816 | 3.952 | 1.00 | 32.12 |
| ATOM | 1822 | N | ARG | 1718 | 35.529 | 0.582 | 5.009 | 1.00 | 31.09 |
| ATOM | 1823 | CA | ARG | 1718 | 34.586 | -0.288 | 5.696 | 1.00 | 32.10 |
| ATOM | 1824 | CB | ARG | 1718 | 34.531 | -1.664 | 5.024 | 1.00 | 31.61 |
| ATOM | 1825 | CG | ARG | 1718 | 34.048 | -1.651 | 3.577 | 1.00 | 31.32 |
| ATOM | 1826 | CD | ARG | 1718 | 32.579 | -1.263 | 3.495 | 1.00 | 29.60 |
| ATOM | 1827 | NE | ARG | 1718 | 32.036 | -1.320 | 2.129 | 1.00 | 24.72 |
| ATOM | 1828 | CZ | ARG | 1718 | 32.103 | -0.324 | 1.243 | 1.00 | 22.01 |
| ATOM | 1829 | NH1 | ARG | 1718 | 32.709 | 0.819 | 1.554 | 1.00 | 19.00 |
| ATOM | 1830 | NH2 | ARG | 1718 | 31.463 | -0.444 | 0.083 | 1.00 | 14.18 |
| ATOM | 1831 | C | ARG | 1718 | 35.042 | -0.438 | 7.164 | 1.00 | 33.81 |
| ATOM | 1832 | O | ARG | 1718 | 36.234 | -0.596 | 7.446 | 1.00 | 34.62 |
| ATOM | 1833 | N | MET | 1719 | 34.084 | -0.372 | 8.085 | 1.00 | 33.99 |
| ATOM | 1834 | CA | MET | 1719 | 34.382 | -0.466 | 9.508 | 1.00 | 32.51 |
| ATOM | 1835 | CB | MET | 1719 | 33.110 | -0.246 | 10.342 | 1.00 | 33.51 |
| ATOM | 1836 | CG | MET | 1719 | 32.513 | 1.155 | 10.200 | 1.00 | 33.69 |
| ATOM | 1837 | SD | MET | 1719 | 31.082 | 1.526 | 11.251 | 1.00 | 37.49 |
| ATOM | 1838 | CE | MET | 1719 | 29.906 | 0.373 | 10.618 | 1.00 | 37.62 |
| ATOM | 1839 | C | MET | 1719 | 35.033 | -1.799 | 9.844 | 1.00 | 32.92 |
| ATOM | 1840 | O | MET | 1719 | 34.900 | -2.772 | 9.098 | 1.00 | 33.67 |
| ATOM | 1841 | N | ASP | 1720 | 35.776 | -1.825 | 10.945 | 1.00 | 35.49 |
| ATOM | 1842 | CA | ASP | 1720 | 36.466 | -3.038 | 11.388 | 1.00 | 36.87 |
| ATOM | 1843 | CB | ASP | 1720 | 37.585 | -2.694 | 12.376 | 1.00 | 41.64 |
| ATOM | 1844 | CG | ASP | 1720 | 38.688 | -1.859 | 11.754 | 1.00 | 46.44 |
| ATOM | 1845 | OD1 | ASP | 1720 | 38.507 | -1.410 | 10.604 | 1.00 | 52.86 |
| ATOM | 1846 | OD2 | ASP | 1720 | 39.740 | -1.650 | 12.422 | 1.00 | 46.76 |
| ATOM | 1847 | C | ASP | 1720 | 35.516 | -4.005 | 12.053 | 1.00 | 34.70 |
| ATOM | 1848 | O | ASP | 1720 | 34.459 | -3.603 | 12.548 | 1.00 | 34.31 |
| ATOM | 1849 | N | LYS | 1721 | 35.937 | -5.265 | 12.132 | 1.00 | 33.39 |
| ATOM | 1850 | CA | LYS | 1721 | 35.119 | -6.297 | 12.755 | 1.00 | 32.68 |
| ATOM | 1851 | CB | LYS | 1721 | 35.692 | -7.690 | 12.500 | 1.00 | 33.55 |
| ATOM | 1852 | CG | LYS | 1721 | 34.834 | -8.791 | 13.119 | 1.00 | 33.62 |
| ATOM | 1853 | CD | LYS | 1721 | 35.336 | -10.158 | 12.771 | 1.00 | 35.77 |
| ATOM | 1854 | CE | LYS | 1721 | 36.082 | -10.747 | 13.931 | 1.00 | 38.73 |
| ATOM | 1855 | NZ | LYS | 1721 | 36.325 | -12.190 | 13.711 | 1.00 | 43.86 |
| ATOM | 1856 | C | LYS | 1721 | 35.034 | -6.107 | 14.240 | 1.00 | 34.61 |
| ATOM | 1857 | O | LYS | 1721 | 36.057 | -5.944 | 14.905 | 1.00 | 37.05 |
| ATOM | 1858 | N | PRO | 1722 | 33.808 | -6.092 | 14.781 | 1.00 | 36.16 |
| ATOM | 1859 | CD | PRO | 1722 | 32.518 | -6.062 | 14.066 | 1.00 | 34.73 |
| ATOM | 1860 | CA | PRO | 1722 | 33.611 | -5.926 | 16.222 | 1.00 | 37.84 |
| ATOM | 1861 | CB | PRO | 1722 | 32.095 | -6.017 | 16.360 | 1.00 | 37.19 |
| ATOM | 1862 | CG | PRO | 1722 | 31.607 | -5.448 | 15.073 | 1.00 | 36.00 |
| ATOM | 1863 | C | PRO | 1722 | 34.266 | -7.109 | 16.950 | 1.00 | 39.95 |
| ATOM | 1864 | O | PRO | 1722 | 34.340 | -8.218 | 16.406 | 1.00 | 38.82 |
| ATOM | 1865 | N | SER | 1723 | 34.783 | -6.884 | 18.150 | 1.00 | 42.36 |
| ATOM | 1866 | CA | SER | 1723 | 35.359 | -7.995 | 18.890 | 1.00 | 45.70 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1867 | CB | SER | 1723 | 36.170 | -7.511 | 20.093 | 1.00 | 47.50 |
| ATOM | 1868 | OG | SER | 1723 | 35.341 | -6.964 | 21.100 | 1.00 | 55.28 |
| ATOM | 1869 | C | SER | 1723 | 34.136 | -8.784 | 19.346 | 1.00 | 46.70 |
| ATOM | 1870 | O | SER | 1723 | 33.037 | -8.224 | 19.477 | 1.00 | 47.27 |
| ATOM | 1871 | N | ASN | 1724 | 34.296 | -10.081 | 19.559 | 1.00 | 47.84 |
| ATOM | 1872 | CA | ASN | 1724 | 33.174 | -10.900 | 19.992 | 1.00 | 51.26 |
| ATOM | 1873 | CB | ASN | 1724 | 32.620 | -10.361 | 21.330 | 1.00 | 57.15 |
| ATOM | 1874 | CG | ASN | 1724 | 33.732 | -10.088 | 22.365 | 1.00 | 61.53 |
| ATOM | 1875 | OD1 | ASN | 1724 | 34.565 | -10.955 | 22.646 | 1.00 | 64.13 |
| ATOM | 1876 | ND2 | ASN | 1724 | 33.763 | -8.867 | 22.912 | 1.00 | 61.69 |
| ATOM | 1877 | C | ASN | 1724 | 32.101 | -10.916 | 18.873 | 1.00 | 50.72 |
| ATOM | 1878 | O | ASN | 1724 | 30.925 | -10.617 | 19.089 | 1.00 | 52.63 |
| ATOM | 1879 | N | CYS | 1725 | 32.564 | -11.193 | 17.663 | 1.00 | 48.01 |
| ATOM | 1880 | CA | CYS | 1725 | 31.719 | -11.295 | 16.478 | 1.00 | 45.16 |
| ATOM | 1881 | CB | CYS | 1725 | 31.603 | -9.929 | 15.788 | 1.00 | 44.77 |
| ATOM | 1882 | SG | CYS | 1725 | 30.605 | -9.929 | 14.272 | 1.00 | 40.74 |
| ATOM | 1883 | C | CYS | 1725 | 32.421 | -12.308 | 15.570 | 1.00 | 41.51 |
| ATOM | 1884 | O | CYS | 1725 | 33.639 | -12.236 | 15.397 | 1.00 | 42.47 |
| ATOM | 1885 | N | THR | 1726 | 31.677 | -13.289 | 15.064 | 1.00 | 37.54 |
| ATOM | 1886 | CA | THR | 1726 | 32.268 | -14.313 | 14.202 | 1.00 | 35.03 |
| ATOM | 1887 | CB | THR | 1726 | 31.308 | -15.500 | 13.993 | 1.00 | 31.87 |
| ATOM | 1888 | OG1 | THR | 1726 | 30.074 | -15.042 | 13.406 | 1.00 | 32.84 |
| ATOM | 1889 | CG2 | THR | 1726 | 31.017 | -16.160 | 15.306 | 1.00 | 29.78 |
| ATOM | 1890 | C | THR | 1726 | 32.678 | -13.770 | 12.845 | 1.00 | 34.76 |
| ATOM | 1891 | O | THR | 1726 | 32.180 | -12.729 | 12.415 | 1.00 | 38.22 |
| ATOM | 1892 | N | ASN | 1727 | 33.596 | -14.450 | 12.175 | 1.00 | 32.47 |
| ATOM | 1893 | CA | ASN | 1727 | 34.009 | -14.024 | 10.842 | 1.00 | 34.75 |
| ATOM | 1894 | CB | ASN | 1727 | 35.167 | -14.872 | 10.308 | 1.00 | 39.77 |
| ATOM | 1895 | CG | ASN | 1727 | 36.464 | -14.591 | 11.026 | 1.00 | 46.09 |
| ATOM | 1896 | OD1 | ASN | 1727 | 37.019 | -13.495 | 10.933 | 1.00 | 49.54 |
| ATOM | 1897 | ND2 | ASN | 1727 | 36.961 | -15.585 | 11.749 | 1.00 | 50.04 |
| ATOM | 1898 | C | ASN | 1727 | 32.825 | -14.147 | 9.905 | 1.00 | 33.38 |
| ATOM | 1899 | O | ASN | 1727 | 32.726 | -13.405 | 8.929 | 1.00 | 34.10 |
| ATOM | 1900 | N | GLU | 1728 | 31.916 | -15.065 | 10.224 | 1.00 | 32.01 |
| ATOM | 1901 | CA | GLU | 1728 | 30.707 | -15.310 | 9.418 | 1.00 | 30.41 |
| ATOM | 1902 | CB | GLU | 1728 | 30.010 | -16.580 | 9.917 | 1.00 | 32.27 |
| ATOM | 1903 | CG | GLU | 1728 | 28.811 | -17.034 | 9.094 | 1.00 | 31.55 |
| ATOM | 1904 | CD | GLU | 1728 | 28.251 | -18.369 | 9.577 | 1.00 | 36.38 |
| ATOM | 1905 | OE1 | GLU | 1728 | 28.415 | -18.694 | 10.777 | 1.00 | 38.35 |
| ATOM | 1906 | OE2 | GLU | 1728 | 27.632 | -19.086 | 8.758 | 1.00 | 36.34 |
| ATOM | 1907 | C | GLU | 1728 | 29.749 | -14.119 | 9.468 | 1.00 | 29.40 |
| ATOM | 1908 | O | GLU | 1728 | 29.231 | -13.679 | 8.438 | 1.00 | 26.23 |
| ATOM | 1909 | N | LEU | 1729 | 29.520 | -13.610 | 10.672 | 1.00 | 29.19 |
| ATOM | 1910 | CA | LEU | 1729 | 28.645 | -12.462 | 10.849 | 1.00 | 30.26 |
| ATOM | 1911 | CB | LEU | 1729 | 28.215 | -12.343 | 12.310 | 1.00 | 30.74 |
| ATOM | 1912 | CG | LEU | 1729 | 27.198 | -13.410 | 12.721 | 1.00 | 31.27 |
| ATOM | 1913 | CD1 | LEU | 1729 | 27.013 | -13.377 | 14.226 | 1.00 | 33.65 |
| ATOM | 1914 | CD2 | LEU | 1729 | 25.865 | -13.161 | 12.010 | 1.00 | 26.16 |
| ATOM | 1915 | C | LEU | 1729 | 29.269 | -11.161 | 10.335 | 1.00 | 28.79 |
| ATOM | 1916 | O | LEU | 1729 | 28.548 | -10.255 | 9.914 | 1.00 | 30.60 |
| ATOM | 1917 | N | TYR | 1730 | 30.594 | -11.069 | 10.363 | 1.00 | 26.64 |
| ATOM | 1918 | CA | TYR | 1730 | 31.281 | -9.881 | 9.844 | 1.00 | 26.47 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1919 | CB | TYR | 1730 | 32.742 | -9.869 | 10.298 | 1.00 | 24.31 |
| ATOM | 1920 | CG | TYR | 1730 | 33.512 | -8.670 | 9.805 | 1.00 | 25.61 |
| ATOM | 1921 | CD1 | TYR | 1730 | 33.029 | -7.373 | 10.016 | 1.00 | 25.68 |
| ATOM | 1922 | CE1 | TYR | 1730 | 33.691 | -6.264 | 9.496 | 1.00 | 23.70 |
| ATOM | 1923 | CD2 | TYR | 1730 | 34.688 | -8.826 | 9.067 | 1.00 | 24.48 |
| ATOM | 1924 | CE2 | TYR | 1730 | 35.361 | -7.719 | 8.537 | 1.00 | 22.61 |
| ATOM | 1925 | CZ | TYR | 1730 | 34.856 | -6.445 | 8.748 | 1.00 | 24.41 |
| ATOM | 1926 | OH | TYR | 1730 | 35.476 | -5.354 | 8.176 | 1.00 | 24.37 |
| ATOM | 1927 | C | TYR | 1730 | 31.186 | -9.902 | 8.301 | 1.00 | 26.06 |
| ATOM | 1928 | O | TYR | 1730 | 30.981 | -8.881 | 7.651 | 1.00 | 23.68 |
| ATOM | 1929 | N | MET | 1731 | 31.347 | -11.084 | 7.727 | 1.00 | 26.60 |
| ATOM | 1930 | CA | MET | 1731 | 31.247 | -11.270 | 6.299 | 1.00 | 29.90 |
| ATOM | 1931 | CB | MET | 1731 | 31.475 | -12.740 | 5.968 | 1.00 | 38.39 |
| ATOM | 1932 | CG | MET | 1731 | 31.076 | -13.157 | 4.577 | 1.00 | 52.98 |
| ATOM | 1933 | SD | MET | 1731 | 31.612 | -14.831 | 4.216 | 1.00 | 69.59 |
| ATOM | 1934 | CE | MET | 1731 | 32.659 | -14.506 | 2.727 | 1.00 | 66.05 |
| ATOM | 1935 | C | MET | 1731 | 29.864 | -10.819 | 5.840 | 1.00 | 29.05 |
| ATOM | 1936 | O | MET | 1731 | 29.720 | -10.194 | 4.791 | 1.00 | 30.94 |
| ATOM | 1937 | N | MET | 1732 | 28.845 | -11.134 | 6.633 | 1.00 | 29.40 |
| ATOM | 1938 | CA | MET | 1732 | 27.475 | -10.743 | 6.328 | 1.00 | 26.97 |
| ATOM | 1939 | CB | MET | 1732 | 26.537 | -11.293 | 7.398 | 1.00 | 25.73 |
| ATOM | 1940 | CG | MET | 1732 | 25.068 | -10.984 | 7.156 | 1.00 | 26.01 |
| ATOM | 1941 | SD | MET | 1732 | 23.980 | -11.637 | 8.407 | 1.00 | 26.97 |
| ATOM | 1942 | CE | MET | 1732 | 23.773 | -13.354 | 7.798 | 1.00 | 21.23 |
| ATOM | 1943 | C | MET | 1732 | 27.387 | -9.220 | 6.271 | 1.00 | 27.49 |
| ATOM | 1944 | O | MET | 1732 | 26.778 | -8.661 | 5.361 | 1.00 | 29.17 |
| ATOM | 1945 | N | MET | 1733 | 27.982 | -8.550 | 7.259 | 1.00 | 27.79 |
| ATOM | 1946 | CA | MET | 1733 | 28.001 | -7.090 | 7.293 | 1.00 | 27.41 |
| ATOM | 1947 | CB | MET | 1733 | 28.797 | -6.587 | 8.484 | 1.00 | 28.84 |
| ATOM | 1948 | CG | MET | 1733 | 28.153 | -6.761 | 9.829 | 1.00 | 32.18 |
| ATOM | 1949 | SD | MET | 1733 | 29.300 | -6.248 | 11.127 | 1.00 | 32.77 |
| ATOM | 1950 | CE | MET | 1733 | 28.850 | -7.423 | 12.399 | 1.00 | 33.03 |
| ATOM | 1951 | C | MET | 1733 | 28.711 | -6.599 | 6.035 | 1.00 | 28.54 |
| ATOM | 1952 | O | MET | 1733 | 28.250 | -5.680 | 5.357 | 1.00 | 30.69 |
| ATOM | 1953 | N | ARG | 1734 | 29.865 | -7.194 | 5.751 | 1.00 | 28.59 |
| ATOM | 1954 | CA | ARG | 1734 | 30.650 | -6.831 | 4.571 | 1.00 | 29.53 |
| ATOM | 1955 | CB | ARG | 1734 | 31.970 | -7.609 | 4.531 | 1.00 | 28.74 |
| ATOM | 1956 | CG | ARG | 1734 | 32.944 | -7.245 | 5.638 | 1.00 | 26.75 |
| ATOM | 1957 | CD | ARG | 1734 | 33.158 | -5.755 | 5.702 | 1.00 | 26.58 |
| ATOM | 1958 | NE | ARG | 1734 | 33.825 | -5.288 | 4.499 | 1.00 | 34.72 |
| ATOM | 1959 | CZ | ARG | 1734 | 35.139 | -5.360 | 4.306 | 1.00 | 37.67 |
| ATOM | 1960 | NH1 | ARG | 1734 | 35.927 | -5.867 | 5.251 | 1.00 | 40.46 |
| ATOM | 1961 | NH2 | ARG | 1734 | 35.663 | -4.986 | 3.147 | 1.00 | 38.11 |
| ATOM | 1962 | C | ARG | 1734 | 29.855 | -7.051 | 3.294 | 1.00 | 28.03 |
| ATOM | 1963 | O | ARG | 1734 | 29.958 | -6.260 | 2.359 | 1.00 | 27.22 |
| ATOM | 1964 | N | ASP | 1735 | 29.071 | -8.130 | 3.260 | 1.00 | 27.81 |
| ATOM | 1965 | CA | ASP | 1735 | 28.212 | -8.436 | 2.103 | 1.00 | 27.27 |
| ATOM | 1966 | CB | ASP | 1735 | 27.608 | -9.835 | 2.216 | 1.00 | 28.62 |
| ATOM | 1967 | CG | ASP | 1735 | 28.638 | -10.932 | 2.075 | 1.00 | 30.15 |
| ATOM | 1968 | OD1 | ASP | 1735 | 29.745 | -10.663 | 1.553 | 1.00 | 31.23 |
| ATOM | 1969 | OD2 | ASP | 1735 | 28.354 | -12.070 | 2.501 | 1.00 | 32.00 |
| ATOM | 1970 | C | ASP | 1735 | 27.099 | -7.400 | 1.971 | 1.00 | 24.78 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1971 | O | ASP | 1735 | 26.714 | -7.068 | 0.852 | 1.00 | 24.52 |
| ATOM | 1972 | N | CYS | 1736 | 26.590 | -6.908 | 3.104 | 1.00 | 24.10 |
| ATOM | 1973 | CA | CYS | 1736 | 25.530 | -5.871 | 3.140 | 1.00 | 25.20 |
| ATOM | 1974 | CB | CYS | 1736 | 24.965 | -5.679 | 4.569 | 1.00 | 23.85 |
| ATOM | 1975 | SG | CYS | 1736 | 23.898 | -7.030 | 5.143 | 1.00 | 18.77 |
| ATOM | 1976 | C | CYS | 1736 | 26.042 | -4.520 | 2.611 | 1.00 | 23.39 |
| ATOM | 1977 | O | CYS | 1736 | 25.276 | -3.718 | 2.070 | 1.00 | 21.76 |
| ATOM | 1978 | N | TRP | 1737 | 27.348 | -4.303 | 2.743 | 1.00 | 23.53 |
| ATOM | 1979 | CA | TRP | 1737 | 27.988 | -3.072 | 2.302 | 1.00 | 21.57 |
| ATOM | 1980 | CB | TRP | 1737 | 29.026 | -2.631 | 3.314 | 1.00 | 18.82 |
| ATOM | 1981 | CG | TRP | 1737 | 28.485 | -2.418 | 4.686 | 1.00 | 19.89 |
| ATOM | 1982 | CD2 | TRP | 1737 | 29.194 | -2.609 | 5.913 | 1.00 | 22.39 |
| ATOM | 1983 | CE2 | TRP | 1737 | 28.329 | -2.213 | 6.959 | 1.00 | 21.78 |
| ATOM | 1984 | CE3 | TRP | 1737 | 30.478 | -3.083 | 6.238 | 1.00 | 23.52 |
| ATOM | 1985 | CD1 | TRP | 1737 | 27.248 | -1.932 | 5.022 | 1.00 | 19.40 |
| ATOM | 1986 | NE1 | TRP | 1737 | 27.147 | -1.805 | 6.383 | 1.00 | 21.52 |
| ATOM | 1987 | CZ2 | TRP | 1737 | 28.705 | -2.270 | 8.319 | 1.00 | 21.85 |
| ATOM | 1988 | CZ3 | TRP | 1737 | 30.857 | -3.134 | 7.583 | 1.00 | 25.30 |
| ATOM | 1989 | CH2 | TRP | 1737 | 29.972 | -2.728 | 8.604 | 1.00 | 26.17 |
| ATOM | 1990 | C | TRP | 1737 | 28.673 | -3.226 | 0.956 | 1.00 | 24.49 |
| ATOM | 1991 | O | TRP | 1737 | 29.648 | -2.519 | 0.670 | 1.00 | 25.09 |
| ATOM | 1992 | N | HIS | 1738 | 28.203 | -4.170 | 0.136 | 1.00 | 25.12 |
| ATOM | 1993 | CA | HIS | 1738 | 28.808 | -4.341 | -1.172 | 1.00 | 22.90 |
| ATOM | 1994 | CB | HIS | 1738 | 28.163 | -5.497 | -1.928 | 1.00 | 23.14 |
| ATOM | 1995 | CG | HIS | 1738 | 29.017 | -6.013 | -3.051 | 1.00 | 23.26 |
| ATOM | 1996 | CD2 | HIS | 1738 | 29.550 | -5.380 | -4.129 | 1.00 | 23.78 |
| ATOM | 1997 | ND1 | HIS | 1738 | 29.492 | -7.308 | -3.104 | 1.00 | 24.91 |
| ATOM | 1998 | CE1 | HIS | 1738 | 30.286 | -7.445 | -4.156 | 1.00 | 25.29 |
| ATOM | 1999 | NE2 | HIS | 1738 | 30.341 | -6.288 | -4.794 | 1.00 | 26.99 |
| ATOM | 2000 | C | HIS | 1738 | 28.670 | -3.024 | -1.958 | 1.00 | 22.92 |
| ATOM | 2001 | O | HIS | 1738 | 27.615 | -2.381 | -1.933 | 1.00 | 20.27 |
| ATOM | 2002 | N | ALA | 1739 | 29.752 | -2.608 | -2.607 | 1.00 | 24.30 |
| ATOM | 2003 | CA | ALA | 1739 | 29.762 | -1.378 | -3.385 | 1.00 | 23.70 |
| ATOM | 2004 | CB | ALA | 1739 | 31.079 | -1.234 | -4.076 | 1.00 | 25.24 |
| ATOM | 2005 | C | ALA | 1739 | 28.645 | -1.391 | -4.416 | 1.00 | 25.37 |
| ATOM | 2006 | O | ALA | 1739 | 27.955 | -0.391 | -4.606 | 1.00 | 27.86 |
| ATOM | 2007 | N | VAL | 1740 | 28.507 | -2.521 | -5.102 | 1.00 | 23.97 |
| ATOM | 2008 | CA | VAL | 1740 | 27.481 | -2.700 | -6.121 | 1.00 | 24.64 |
| ATOM | 2009 | CB | VAL | 1740 | 27.966 | -3.698 | -7.206 | 1.00 | 26.39 |
| ATOM | 2010 | CG1 | VAL | 1740 | 27.013 | -3.757 | -8.360 | 1.00 | 22.65 |
| ATOM | 2011 | CG2 | VAL | 1740 | 29.308 | -3.260 | -7.720 | 1.00 | 27.43 |
| ATOM | 2012 | C | VAL | 1740 | 26.170 | -3.209 | -5.481 | 1.00 | 23.97 |
| ATOM | 2013 | O | VAL | 1740 | 26.126 | -4.347 | -4.978 | 1.00 | 24.14 |
| ATOM | 2014 | N | PRO | 1741 | 25.090 | -2.397 | -5.545 | 1.00 | 22.77 |
| ATOM | 2015 | CD | PRO | 1741 | 25.074 | -1.093 | -6.237 | 1.00 | 17.82 |
| ATOM | 2016 | CA | PRO | 1741 | 23.763 | -2.695 | -4.980 | 1.00 | 23.22 |
| ATOM | 2017 | CB | PRO | 1741 | 22.891 | -1.554 | -5.526 | 1.00 | 18.19 |
| ATOM | 2018 | CG | PRO | 1741 | 23.866 | -0.419 | -5.647 | 1.00 | 15.09 |
| ATOM | 2019 | C | PRO | 1741 | 23.189 | -4.074 | -5.343 | 1.00 | 23.26 |
| ATOM | 2020 | O | PRO | 1741 | 22.700 | -4.788 | -4.462 | 1.00 | 22.42 |
| ATOM | 2021 | N | SER | 1742 | 23.335 | -4.473 | -6.615 | 1.00 | 23.49 |
| ATOM | 2022 | CA | SER | 1742 | 22.826 | -5.754 | -7.119 | 1.00 | 23.17 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2023 | CB | SER | 1742 | 22.956 | -5.808 | -8.641 | 1.00 | 23.67 |
| ATOM | 2024 | OG | SER | 1742 | 24.324 | -5.891 | -9.023 | 1.00 | 26.64 |
| ATOM | 2025 | C | SER | 1742 | 23.524 | -6.984 | -6.545 | 1.00 | 23.09 |
| ATOM | 2026 | O | SER | 1742 | 22.993 | -8.104 | -6.603 | 1.00 | 21.90 |
| ATOM | 2027 | N | GLN | 1743 | 24.719 | -6.782 | -5.997 | 1.00 | 23.62 |
| ATOM | 2028 | CA | GLN | 1743 | 25.466 | -7.895 | -5.416 | 1.00 | 23.26 |
| ATOM | 2029 | CB | GLN | 1743 | 26.953 | -7.754 | -5.702 | 1.00 | 24.32 |
| ATOM | 2030 | CG | GLN | 1743 | 27.255 | -7.828 | -7.170 | 1.00 | 23.04 |
| ATOM | 2031 | CD | GLN | 1743 | 26.684 | -9.076 | -7.810 | 1.00 | 24.83 |
| ATOM | 2032 | OE1 | GLN | 1743 | 27.176 | -10.178 | -7.584 | 1.00 | 21.07 |
| ATOM | 2033 | NE2 | GLN | 1743 | 25.647 | -8.907 | -8.625 | 1.00 | 22.66 |
| ATOM | 2034 | C | GLN | 1743 | 25.227 | -8.121 | -3.927 | 1.00 | 23.85 |
| ATOM | 2035 | O | GLN | 1743 | 25.744 | -9.083 | -3.366 | 1.00 | 25.36 |
| ATOM | 2036 | N | ARG | 1744 | 24.458 | -7.240 | -3.290 | 1.00 | 22.69 |
| ATOM | 2037 | CA | ARG | 1744 | 24.155 | -7.395 | -1.868 | 1.00 | 21.65 |
| ATOM | 2038 | CB | ARG | 1744 | 23.635 | -6.087 | -1.277 | 1.00 | 21.22 |
| ATOM | 2039 | CG | ARG | 1744 | 24.623 | -4.962 | -1.342 | 1.00 | 21.63 |
| ATOM | 2040 | CD | ARG | 1744 | 24.013 | -3.656 | -0.863 | 1.00 | 19.06 |
| ATOM | 2041 | NE | ARG | 1744 | 24.869 | -2.563 | -1.318 | 1.00 | 24.44 |
| ATOM | 2042 | CZ | ARG | 1744 | 24.461 | -1.322 | -1.564 | 1.00 | 22.49 |
| ATOM | 2043 | NH1 | ARG | 1744 | 23.184 | -0.972 | -1.378 | 1.00 | 18.95 |
| ATOM | 2044 | NH2 | ARG | 1744 | 25.337 | -0.438 | -2.034 | 1.00 | 22.19 |
| ATOM | 2045 | C | ARG | 1744 | 23.095 | -8.470 | -1.712 | 1.00 | 22.45 |
| ATOM | 2046 | O | ARG | 1744 | 22.363 | -8.772 | -2.654 | 1.00 | 25.62 |
| ATOM | 2047 | N | PRO | 1745 | 23.065 | -9.139 | -0.559 | 1.00 | 21.78 |
| ATOM | 2048 | CD | PRO | 1745 | 24.025 | -9.114 | 0.563 | 1.00 | 21.02 |
| ATOM | 2049 | CA | PRO | 1745 | 22.057 | -10.175 | -0.362 | 1.00 | 20.99 |
| ATOM | 2050 | CB | PRO | 1745 | 22.532 | -10.879 | 0.919 | 1.00 | 21.12 |
| ATOM | 2051 | CG | PRO | 1745 | 23.240 | -9.777 | 1.676 | 1.00 | 19.86 |
| ATOM | 2052 | C | PRO | 1745 | 20.726 | -9.485 | -0.146 | 1.00 | 22.18 |
| ATOM | 2053 | O | PRO | 1745 | 20.680 | -8.281 | 0.128 | 1.00 | 23.04 |
| ATOM | 2054 | N | THR | 1746 | 19.646 | -10.236 | -0.297 | 1.00 | 19.31 |
| ATOM | 2055 | CA | THR | 1746 | 18.335 | -9.689 | -0.085 | 1.00 | 19.12 |
| ATOM | 2056 | CB | THR | 1746 | 17.307 | -10.334 | -1.045 | 1.00 | 19.86 |
| ATOM | 2057 | OG1 | THR | 1746 | 17.299 | -11.763 | -0.886 | 1.00 | 22.54 |
| ATOM | 2058 | CG2 | THR | 1746 | 17.668 | -10.002 | -2.479 | 1.00 | 22.97 |
| ATOM | 2059 | C | THR | 1746 | 17.961 | -9.975 | 1.367 | 1.00 | 19.91 |
| ATOM | 2060 | O | THR | 1746 | 18.676 | -10.711 | 2.058 | 1.00 | 19.93 |
| ATOM | 2061 | N | PHE | 1747 | 16.884 | -9.381 | 1.855 | 1.00 | 21.80 |
| ATOM | 2062 | CA | PHE | 1747 | 16.456 | -9.678 | 3.224 | 1.00 | 23.46 |
| ATOM | 2063 | CB | PHE | 1747 | 15.353 | -8.720 | 3.686 | 1.00 | 21.84 |
| ATOM | 2064 | CG | PHE | 1747 | 15.872 | -7.368 | 4.082 | 1.00 | 24.84 |
| ATOM | 2065 | CD1 | PHE | 1747 | 16.627 | -7.207 | 5.237 | 1.00 | 22.23 |
| ATOM | 2066 | CD2 | PHE | 1747 | 15.611 | -6.248 | 3.293 | 1.00 | 22.97 |
| ATOM | 2067 | CE1 | PHE | 1747 | 17.124 | -5.944 | 5.598 | 1.00 | 19.42 |
| ATOM | 2068 | CE2 | PHE | 1747 | 16.111 | -4.991 | 3.646 | 1.00 | 17.14 |
| ATOM | 2069 | CZ | PHE | 1747 | 16.862 | -4.846 | 4.801 | 1.00 | 18.02 |
| ATOM | 2070 | C | PHE | 1747 | 15.992 | -11.133 | 3.295 | 1.00 | 22.28 |
| ATOM | 2071 | O | PHE | 1747 | 16.189 | -11.796 | 4.304 | 1.00 | 23.76 |
| ATOM | 2072 | N | LYS | 1748 | 15.430 | -11.632 | 2.199 | 1.00 | 23.46 |
| ATOM | 2073 | CA | LYS | 1748 | 14.971 | -13.014 | 2.140 | 1.00 | 25.84 |
| ATOM | 2074 | CB | LYS | 1748 | 14.344 | -13.327 | 0.782 | 1.00 | 26.89 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2075 | CG | LYS | 1748 | 14.061 | -14.793 | 0.583 | 1.00 | 31.07 |
| ATOM | 2076 | CD | LYS | 1748 | 13.714 | -15.064 | -0.861 | 1.00 | 37.82 |
| ATOM | 2077 | CE | LYS | 1748 | 13.231 | -16.493 | -1.068 | 1.00 | 44.36 |
| ATOM | 2078 | NZ | LYS | 1748 | 12.027 | -16.782 | -0.235 | 1.00 | 50.16 |
| ATOM | 2079 | C | LYS | 1748 | 16.160 | -13.949 | 2.393 | 1.00 | 27.27 |
| ATOM | 2080 | O | LYS | 1748 | 16.067 | -14.877 | 3.202 | 1.00 | 27.87 |
| ATOM | 2081 | N | GLN | 1749 | 17.288 | -13.674 | 1.730 | 1.00 | 25.64 |
| ATOM | 2082 | CA | GLN | 1749 | 18.507 | -14.457 | 1.903 | 1.00 | 24.32 |
| ATOM | 2083 | CB | GLN | 1749 | 19.608 | -13.938 | 0.983 | 1.00 | 28.87 |
| ATOM | 2084 | CG | GLN | 1749 | 19.343 | -14.049 | -0.496 | 1.00 | 36.24 |
| ATOM | 2085 | CD | GLN | 1749 | 20.437 | -13.374 | -1.318 | 1.00 | 41.30 |
| ATOM | 2086 | OE1 | GLN | 1749 | 20.173 | -12.422 | -2.044 | 1.00 | 38.35 |
| ATOM | 2087 | NE2 | GLN | 1749 | 21.683 | -13.861 | -1.190 | 1.00 | 45.38 |
| ATOM | 2088 | C | GLN | 1749 | 19.002 | -14.310 | 3.346 | 1.00 | 22.89 |
| ATOM | 2089 | O | GLN | 1749 | 19.302 | -15.305 | 4.008 | 1.00 | 22.55 |
| ATOM | 2090 | N | LEU | 1750 | 19.114 | -13.064 | 3.813 | 1.00 | 20.89 |
| ATOM | 2091 | CA | LEU | 1750 | 19.570 | -12.776 | 5.167 | 1.00 | 21.44 |
| ATOM | 2092 | CB | LEU | 1750 | 19.471 | -11.282 | 5.462 | 1.00 | 19.53 |
| ATOM | 2093 | CG | LEU | 1750 | 20.432 | -10.400 | 4.663 | 1.00 | 19.14 |
| ATOM | 2094 | CD1 | LEU | 1750 | 20.069 | -8.919 | 4.816 | 1.00 | 14.53 |
| ATOM | 2095 | CD2 | LEU | 1750 | 21.863 | -10.685 | 5.106 | 1.00 | 16.18 |
| ATOM | 2096 | C | LEU | 1750 | 18.776 | -13.538 | 6.208 | 1.00 | 22.98 |
| ATOM | 2097 | O | LEU | 1750 | 19.335 | -14.057 | 7.183 | 1.00 | 23.12 |
| ATOM | 2098 | N | VAL | 1751 | 17.465 | -13.586 | 6.020 | 1.00 | 23.48 |
| ATOM | 2099 | CA | VAL | 1751 | 16.610 | -14.292 | 6.945 | 1.00 | 23.21 |
| ATOM | 2100 | CB | VAL | 1751 | 15.132 | -14.075 | 6.590 | 1.00 | 20.94 |
| ATOM | 2101 | CG1 | VAL | 1751 | 14.268 | -15.008 | 7.375 | 1.00 | 21.67 |
| ATOM | 2102 | CG2 | VAL | 1751 | 14.730 | -12.649 | 6.929 | 1.00 | 20.32 |
| ATOM | 2103 | C | VAL | 1751 | 16.974 | -15.774 | 6.990 | 1.00 | 26.13 |
| ATOM | 2104 | O | VAL | 1751 | 17.030 | -16.379 | 8.058 | 1.00 | 26.35 |
| ATOM | 2105 | N | GLU | 1752 | 17.260 | -16.348 | 5.831 | 1.00 | 30.05 |
| ATOM | 2106 | CA | GLU | 1752 | 17.632 | -17.747 | 5.778 | 1.00 | 32.54 |
| ATOM | 2107 | CB | GLU | 1752 | 17.695 | -18.221 | 4.338 | 1.00 | 38.54 |
| ATOM | 2108 | CG | GLU | 1752 | 16.322 | -18.226 | 3.673 | 1.00 | 50.06 |
| ATOM | 2109 | CD | GLU | 1752 | 16.333 | -18.759 | 2.247 | 1.00 | 56.55 |
| ATOM | 2110 | OE1 | GLU | 1752 | 15.365 | -18.480 | 1.507 | 1.00 | 61.63 |
| ATOM | 2111 | OE2 | GLU | 1752 | 17.303 | -19.466 | 1.875 | 1.00 | 59.57 |
| ATOM | 2112 | C | GLU | 1752 | 18.974 | -17.965 | 6.486 | 1.00 | 31.62 |
| ATOM | 2113 | O | GLU | 1752 | 19.113 | -18.858 | 7.322 | 1.00 | 29.63 |
| ATOM | 2114 | N | ASP | 1753 | 19.938 | -17.103 | 6.193 | 1.00 | 30.74 |
| ATOM | 2115 | CA | ASP | 1753 | 21.246 | -17.211 | 6.807 | 1.00 | 31.00 |
| ATOM | 2116 | CB | ASP | 1753 | 22.209 | -16.181 | 6.203 | 1.00 | 31.47 |
| ATOM | 2117 | CG | ASP | 1753 | 22.445 | -16.390 | 4.710 | 1.00 | 35.82 |
| ATOM | 2118 | OD1 | ASP | 1753 | 22.396 | -17.549 | 4.248 | 1.00 | 36.78 |
| ATOM | 2119 | OD2 | ASP | 1753 | 22.671 | -15.396 | 3.992 | 1.00 | 41.04 |
| ATOM | 2120 | C | ASP | 1753 | 21.158 | -17.058 | 8.314 | 1.00 | 28.94 |
| ATOM | 2121 | O | ASP | 1753 | 21.597 | -17.933 | 9.059 | 1.00 | 29.91 |
| ATOM | 2122 | N | LEU | 1754 | 20.526 | -15.984 | 8.764 | 1.00 | 28.33 |
| ATOM | 2123 | CA | LEU | 1754 | 20.386 | -15.731 | 10.199 | 1.00 | 26.88 |
| ATOM | 2124 | CB | LEU | 1754 | 19.724 | -14.372 | 10.457 | 1.00 | 19.82 |
| ATOM | 2125 | CG | LEU | 1754 | 20.737 | -13.269 | 10.154 | 1.00 | 20.90 |
| ATOM | 2126 | CD1 | LEU | 1754 | 20.074 | -11.886 | 9.995 | 1.00 | 14.83 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2127 | CD2 | LEU | 1754 | 21.831 | -13.308 | 11.240 | 1.00 | 16.39 |
| ATOM | 2128 | C | LEU | 1754 | 19.645 | -16.861 | 10.896 | 1.00 | 29.18 |
| ATOM | 2129 | O | LEU | 1754 | 20.030 | -17.262 | 11.986 | 1.00 | 30.55 |
| ATOM | 2130 | N | ASP | 1755 | 18.638 | -17.421 | 10.238 | 1.00 | 31.65 |
| ATOM | 2131 | CA | ASP | 1755 | 17.892 | -18.517 | 10.822 | 1.00 | 31.78 |
| ATOM | 2132 | CB | ASP | 1755 | 16.723 | -18.900 | 9.928 | 1.00 | 34.57 |
| ATOM | 2133 | CG | ASP | 1755 | 15.876 | -19.997 | 10.533 | 1.00 | 38.29 |
| ATOM | 2134 | OD1 | ASP | 1755 | 15.410 | -19.844 | 11.677 | 1.00 | 45.68 |
| ATOM | 2135 | OD2 | ASP | 1755 | 15.685 | -21.031 | 9.878 | 1.00 | 43.09 |
| ATOM | 2136 | C | ASP | 1755 | 18.801 | -19.713 | 11.034 | 1.00 | 33.50 |
| ATOM | 2137 | O | ASP | 1755 | 18.665 | -20.428 | 12.025 | 1.00 | 34.39 |
| ATOM | 2138 | N | ARG | 1756 | 19.738 | -19.907 | 10.107 | 1.00 | 35.51 |
| ATOM | 2139 | CA | ARG | 1756 | 20.700 | -21.004 | 10.169 | 1.00 | 35.33 |
| ATOM | 2140 | CB | ARG | 1756 | 21.417 | -21.125 | 8.825 | 1.00 | 38.41 |
| ATOM | 2141 | CG | ARG | 1756 | 22.522 | -22.181 | 8.759 | 1.00 | 40.99 |
| ATOM | 2142 | CD | ARG | 1756 | 23.181 | -22.223 | 7.376 | 1.00 | 44.60 |
| ATOM | 2143 | NE | ARG | 1756 | 23.676 | -20.917 | 6.916 | 1.00 | 49.55 |
| ATOM | 2144 | CZ | ARG | 1756 | 24.795 | -20.338 | 7.349 | 1.00 | 53.56 |
| ATOM | 2145 | NH1 | ARG | 1756 | 25.556 | -20.937 | 8.266 | 1.00 | 53.25 |
| ATOM | 2146 | NH2 | ARG | 1756 | 25.165 | -19.163 | 6.853 | 1.00 | 55.72 |
| ATOM | 2147 | C | ARG | 1756 | 21.719 | -20.754 | 11.275 | 1.00 | 35.01 |
| ATOM | 2148 | O | ARG | 1756 | 22.000 | -21.632 | 12.088 | 1.00 | 34.86 |
| ATOM | 2149 | N | ILE | 1757 | 22.244 | -19.536 | 11.314 | 1.00 | 35.06 |
| ATOM | 2150 | CA | ILE | 1757 | 23.242 | -19.153 | 12.302 | 1.00 | 35.25 |
| ATOM | 2151 | CB | ILE | 1757 | 23.847 | -17.753 | 11.984 | 1.00 | 34.59 |
| ATOM | 2152 | CG2 | ILE | 1757 | 24.915 | -17.401 | 12.995 | 1.00 | 32.98 |
| ATOM | 2153 | CG1 | ILE | 1757 | 24.481 | -17.757 | 10.586 | 1.00 | 33.64 |
| ATOM | 2154 | CD1 | ILE | 1757 | 24.812 | -16.387 | 10.032 | 1.00 | 28.79 |
| ATOM | 2155 | C | ILE | 1757 | 22.673 | -19.182 | 13.716 | 1.00 | 36.74 |
| ATOM | 2156 | O | ILE | 1757 | 23.283 | -19.764 | 14.601 | 1.00 | 36.60 |
| ATOM | 2157 | N | VAL | 1758 | 21.489 | -18.608 | 13.917 | 1.00 | 39.16 |
| ATOM | 2158 | CA | VAL | 1758 | 20.854 | -18.589 | 15.243 | 1.00 | 41.06 |
| ATOM | 2159 | CB | VAL | 1758 | 19.378 | -18.104 | 15.165 | 1.00 | 38.77 |
| ATOM | 2160 | CG1 | VAL | 1758 | 18.715 | -18.183 | 16.530 | 1.00 | 38.72 |
| ATOM | 2161 | CG2 | VAL | 1758 | 19.309 | -16.670 | 14.651 | 1.00 | 39.49 |
| ATOM | 2162 | C | VAL | 1758 | 20.885 | -19.986 | 15.850 | 1.00 | 43.92 |
| ATOM | 2163 | O | VAL | 1758 | 21.403 | -20.182 | 16.954 | 1.00 | 46.90 |
| ATOM | 2164 | N | ALA | 1759 | 20.370 | -20.957 | 15.098 | 1.00 | 43.96 |
| ATOM | 2165 | CA | ALA | 1759 | 20.325 | -22.354 | 15.528 | 1.00 | 43.47 |
| ATOM | 2166 | CB | ALA | 1759 | 19.653 | -23.197 | 14.460 | 1.00 | 42.26 |
| ATOM | 2167 | C | ALA | 1759 | 21.693 | -22.953 | 15.890 | 1.00 | 44.02 |
| ATOM | 2168 | O | ALA | 1759 | 21.780 | -23.872 | 16.697 | 1.00 | 45.94 |
| ATOM | 2169 | N | LEU | 1760 | 22.750 | -22.465 | 15.255 | 1.00 | 45.07 |
| ATOM | 2170 | CA | LEU | 1760 | 24.095 | -22.949 | 15.514 | 1.00 | 46.72 |
| ATOM | 2171 | CB | LEU | 1760 | 24.899 | -22.900 | 14.225 | 1.00 | 48.22 |
| ATOM | 2172 | CG | LEU | 1760 | 24.279 | -23.645 | 13.053 | 1.00 | 51.98 |
| ATOM | 2173 | CD1 | LEU | 1760 | 25.016 | -23.279 | 11.778 | 1.00 | 56.19 |
| ATOM | 2174 | CD2 | LEU | 1760 | 24.327 | -25.136 | 13.313 | 1.00 | 52.82 |
| ATOM | 2175 | C | LEU | 1760 | 24.811 | -22.118 | 16.578 | 1.00 | 47.59 |
| ATOM | 2176 | O | LEU | 1760 | 25.935 | -22.432 | 16.986 | 1.00 | 44.63 |
| ATOM | 2177 | N | THR | 1761 | 24.181 | -21.031 | 17.004 | 1.00 | 49.32 |
| ATOM | 2178 | CA | THR | 1761 | 24.791 | -20.166 | 17.987 | 1.00 | 50.15 |

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ATOM   2179  CB   THR  1761      24.309 -18.707  17.811  1.00 49.78
ATOM   2180  OG1  THR  1761      24.650 -18.262  16.489  1.00 49.83
ATOM   2181  CG2  THR  1761      24.997 -17.793  18.809  1.00 49.37
ATOM   2182  C    THR  1761      24.643 -20.655  19.426  1.00 51.84
ATOM   2183  O    THR  1761      23.565 -21.064  19.866  1.00 51.38
ATOM   2184  N    SER  1762      25.761 -20.622  20.143  1.00 53.45
ATOM   2185  CA   SER  1762      25.835 -21.042  21.533  1.00 53.79
ATOM   2186  CB   SER  1762      27.301 -21.039  21.969  1.00 58.33
ATOM   2187  OG   SER  1762      27.502 -21.759  23.173  1.00 63.27
ATOM   2188  C    SER  1762      25.033 -20.081  22.403  1.00 50.43
ATOM   2189  O    SER  1762      25.193 -18.856  22.301  1.00 48.42
ATOM   2190  N    ALA   461      79.680  25.808  14.502  1.00 57.40
ATOM   2191  CA   ALA   461      79.609  24.651  13.610  1.00 53.47
ATOM   2192  CB   ALA   461      78.307  23.875  13.860  1.00 54.34
ATOM   2193  C    ALA   461      79.707  25.105  12.151  1.00 49.53
ATOM   2194  O    ALA   461      79.739  24.289  11.243  1.00 48.04
ATOM   2195  N    ALA   462      79.814  26.417  11.957  1.00 46.57
ATOM   2196  CA   ALA   462      79.919  27.014  10.634  1.00 43.66
ATOM   2197  CB   ALA   462      80.034  28.532  10.750  1.00 43.87
ATOM   2198  C    ALA   462      81.074  26.461   9.806  1.00 39.75
ATOM   2199  O    ALA   462      80.869  26.036   8.673  1.00 36.18
ATOM   2200  N    TYR   463      82.279  26.449  10.383  1.00 37.82
ATOM   2201  CA   TYR   463      83.477  25.959   9.686  1.00 36.88
ATOM   2202  CB   TYR   463      84.615  26.968   9.765  1.00 39.12
ATOM   2203  CG   TYR   463      84.372  28.176   8.894  1.00 45.68
ATOM   2204  CD1  TYR   463      84.071  29.422   9.456  1.00 46.07
ATOM   2205  CE1  TYR   463      83.783  30.518   8.652  1.00 48.07
ATOM   2206  CD2  TYR   463      84.384  28.064   7.501  1.00 47.80
ATOM   2207  CE2  TYR   463      84.096  29.154   6.690  1.00 45.55
ATOM   2208  CZ   TYR   463      83.796  30.372   7.271  1.00 47.44
ATOM   2209  OH   TYR   463      83.491  31.442   6.476  1.00 49.77
ATOM   2210  C    TYR   463      83.988  24.579  10.024  1.00 34.97
ATOM   2211  O    TYR   463      84.605  23.947   9.175  1.00 35.48
ATOM   2212  N    GLU   464      83.761  24.109  11.244  1.00 34.33
ATOM   2213  CA   GLU   464      84.224  22.769  11.630  1.00 36.96
ATOM   2214  CB   GLU   464      85.725  22.790  11.901  1.00 41.01
ATOM   2215  CG   GLU   464      86.123  23.764  12.991  1.00 45.91
ATOM   2216  CD   GLU   464      87.619  24.009  13.075  1.00 53.97
ATOM   2217  OE1  GLU   464      88.013  24.922  13.835  1.00 58.84
ATOM   2218  OE2  GLU   464      88.400  23.311  12.383  1.00 56.78
ATOM   2219  C    GLU   464      83.517  22.294  12.875  1.00 34.98
ATOM   2220  O    GLU   464      83.252  23.106  13.763  1.00 35.30
ATOM   2221  N    LEU   465      83.193  21.003  12.939  1.00 33.52
ATOM   2222  CA   LEU   465      82.527  20.449  14.121  1.00 35.65
ATOM   2223  CB   LEU   465      81.520  19.348  13.762  1.00 32.97
ATOM   2224  CG   LEU   465      80.488  19.538  12.651  1.00 33.16
ATOM   2225  CD1  LEU   465      79.356  18.544  12.911  1.00 27.30
ATOM   2226  CD2  LEU   465      79.983  20.981  12.596  1.00 29.96
ATOM   2227  C    LEU   465      83.572  19.862  15.058  1.00 38.14
ATOM   2228  O    LEU   465      84.707  19.573  14.642  1.00 35.58
ATOM   2229  N    PRO   466      83.215  19.684  16.338  1.00 39.91
ATOM   2230  CD   PRO   466      81.929  20.073  16.942  1.00 42.38
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2231 | CA | PRO | 466 | 84.118 | 19.126 | 17.348 | 1.00 | 40.82 |
| ATOM | 2232 | CB | PRO | 466 | 83.264 | 19.131 | 18.611 | 1.00 | 41.62 |
| ATOM | 2233 | CG | PRO | 466 | 82.327 | 20.294 | 18.380 | 1.00 | 45.42 |
| ATOM | 2234 | C | PRO | 466 | 84.475 | 17.707 | 16.976 | 1.00 | 41.29 |
| ATOM | 2235 | O | PRO | 466 | 83.681 | 16.996 | 16.361 | 1.00 | 40.64 |
| ATOM | 2236 | N | GLU | 467 | 85.664 | 17.292 | 17.370 | 1.00 | 43.54 |
| ATOM | 2237 | CA | GLU | 467 | 86.106 | 15.950 | 17.065 | 1.00 | 47.01 |
| ATOM | 2238 | CB | GLU | 467 | 87.569 | 15.955 | 16.627 | 1.00 | 50.95 |
| ATOM | 2239 | CG | GLU | 467 | 88.000 | 14.641 | 15.990 | 1.00 | 59.47 |
| ATOM | 2240 | CD | GLU | 467 | 89.372 | 14.700 | 15.334 | 1.00 | 63.95 |
| ATOM | 2241 | OE1 | GLU | 467 | 90.123 | 15.688 | 15.538 | 1.00 | 62.08 |
| ATOM | 2242 | OE2 | GLU | 467 | 89.697 | 13.736 | 14.606 | 1.00 | 66.76 |
| ATOM | 2243 | C | GLU | 467 | 85.892 | 14.993 | 18.233 | 1.00 | 44.81 |
| ATOM | 2244 | O | GLU | 467 | 85.988 | 15.386 | 19.397 | 1.00 | 45.53 |
| ATOM | 2245 | N | ASP | 468 | 85.572 | 13.751 | 17.906 | 1.00 | 43.85 |
| ATOM | 2246 | CA | ASP | 468 | 85.357 | 12.708 | 18.903 | 1.00 | 43.44 |
| ATOM | 2247 | CB | ASP | 468 | 83.872 | 12.582 | 19.247 | 1.00 | 43.33 |
| ATOM | 2248 | CG | ASP | 468 | 83.611 | 11.659 | 20.420 | 1.00 | 44.52 |
| ATOM | 2249 | OD1 | ASP | 468 | 82.452 | 11.613 | 20.888 | 1.00 | 48.19 |
| ATOM | 2250 | OD2 | ASP | 468 | 84.557 | 10.985 | 20.877 | 1.00 | 42.43 |
| ATOM | 2251 | C | ASP | 468 | 85.887 | 11.411 | 18.299 | 1.00 | 42.37 |
| ATOM | 2252 | O | ASP | 468 | 85.158 | 10.644 | 17.669 | 1.00 | 43.22 |
| ATOM | 2253 | N | PRO | 469 | 87.194 | 11.182 | 18.433 | 1.00 | 40.72 |
| ATOM | 2254 | CD | PRO | 469 | 88.167 | 12.102 | 19.045 | 1.00 | 40.30 |
| ATOM | 2255 | CA | PRO | 469 | 87.861 | 9.992 | 17.909 | 1.00 | 39.00 |
| ATOM | 2256 | CB | PRO | 469 | 89.228 | 10.078 | 18.570 | 1.00 | 39.03 |
| ATOM | 2257 | CG | PRO | 469 | 89.484 | 11.564 | 18.551 | 1.00 | 38.11 |
| ATOM | 2258 | C | PRO | 469 | 87.173 | 8.663 | 18.229 | 1.00 | 39.37 |
| ATOM | 2259 | O | PRO | 469 | 87.235 | 7.718 | 17.442 | 1.00 | 39.27 |
| ATOM | 2260 | N | ARG | 470 | 86.497 | 8.596 | 19.371 | 1.00 | 39.93 |
| ATOM | 2261 | CA | ARG | 470 | 85.814 | 7.374 | 19.770 | 1.00 | 42.32 |
| ATOM | 2262 | CB | ARG | 470 | 85.030 | 7.614 | 21.062 | 1.00 | 46.12 |
| ATOM | 2263 | CG | ARG | 470 | 85.766 | 8.370 | 22.149 | 1.00 | 50.76 |
| ATOM | 2264 | CD | ARG | 470 | 84.839 | 8.592 | 23.344 | 1.00 | 52.76 |
| ATOM | 2265 | NE | ARG | 470 | 83.649 | 9.362 | 22.991 | 1.00 | 54.47 |
| ATOM | 2266 | CZ | ARG | 470 | 82.770 | 9.823 | 23.873 | 1.00 | 59.36 |
| ATOM | 2267 | NH1 | ARG | 470 | 82.945 | 9.597 | 25.169 | 1.00 | 61.19 |
| ATOM | 2268 | NH2 | ARG | 470 | 81.712 | 10.508 | 23.455 | 1.00 | 62.88 |
| ATOM | 2269 | C | ARG | 470 | 84.814 | 6.896 | 18.721 | 1.00 | 42.79 |
| ATOM | 2270 | O | ARG | 470 | 84.670 | 5.700 | 18.504 | 1.00 | 45.63 |
| ATOM | 2271 | N | TRP | 471 | 84.139 | 7.844 | 18.078 | 1.00 | 41.98 |
| ATOM | 2272 | CA | TRP | 471 | 83.100 | 7.542 | 17.093 | 1.00 | 38.34 |
| ATOM | 2273 | CB | TRP | 471 | 81.844 | 8.307 | 17.451 | 1.00 | 35.68 |
| ATOM | 2274 | CG | TRP | 471 | 81.195 | 7.794 | 18.670 | 1.00 | 37.42 |
| ATOM | 2275 | CD2 | TRP | 471 | 80.388 | 6.614 | 18.772 | 1.00 | 37.19 |
| ATOM | 2276 | CE2 | TRP | 471 | 79.961 | 6.513 | 20.112 | 1.00 | 36.99 |
| ATOM | 2277 | CE3 | TRP | 471 | 79.987 | 5.626 | 17.855 | 1.00 | 37.80 |
| ATOM | 2278 | CD1 | TRP | 471 | 81.223 | 8.350 | 19.923 | 1.00 | 33.34 |
| ATOM | 2279 | NE1 | TRP | 471 | 80.486 | 7.583 | 20.794 | 1.00 | 34.46 |
| ATOM | 2280 | CZ2 | TRP | 471 | 79.150 | 5.464 | 20.559 | 1.00 | 38.31 |
| ATOM | 2281 | CZ3 | TRP | 471 | 79.180 | 4.578 | 18.303 | 1.00 | 36.97 |
| ATOM | 2282 | CH2 | TRP | 471 | 78.772 | 4.506 | 19.638 | 1.00 | 36.14 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2283 | C | TRP | 471 | 83.409 | 7.830 | 15.641 | 1.00 | 38.26 |
| ATOM | 2284 | O | TRP | 471 | 82.655 | 7.430 | 14.749 | 1.00 | 38.72 |
| ATOM | 2285 | N | GLU | 472 | 84.478 | 8.569 | 15.397 | 1.00 | 37.71 |
| ATOM | 2286 | CA | GLU | 472 | 84.839 | 8.951 | 14.041 | 1.00 | 38.43 |
| ATOM | 2287 | CB | GLU | 472 | 86.014 | 9.924 | 14.087 | 1.00 | 37.56 |
| ATOM | 2288 | CG | GLU | 472 | 86.146 | 10.835 | 12.871 | 1.00 | 37.26 |
| ATOM | 2289 | CD | GLU | 472 | 84.930 | 11.728 | 12.625 | 1.00 | 39.02 |
| ATOM | 2290 | OE1 | GLU | 472 | 84.361 | 12.301 | 13.571 | 1.00 | 40.26 |
| ATOM | 2291 | OE2 | GLU | 472 | 84.568 | 11.879 | 11.445 | 1.00 | 39.35 |
| ATOM | 2292 | C | GLU | 472 | 85.135 | 7.806 | 13.069 | 1.00 | 38.32 |
| ATOM | 2293 | O | GLU | 472 | 85.872 | 6.875 | 13.386 | 1.00 | 38.11 |
| ATOM | 2294 | N | LEU | 473 | 84.535 | 7.884 | 11.883 | 1.00 | 38.44 |
| ATOM | 2295 | CA | LEU | 473 | 84.775 | 6.893 | 10.848 | 1.00 | 37.19 |
| ATOM | 2296 | CB | LEU | 473 | 83.505 | 6.112 | 10.511 | 1.00 | 35.38 |
| ATOM | 2297 | CG | LEU | 473 | 83.805 | 4.910 | 9.599 | 1.00 | 36.49 |
| ATOM | 2298 | CD1 | LEU | 473 | 84.365 | 3.748 | 10.406 | 1.00 | 34.47 |
| ATOM | 2299 | CD2 | LEU | 473 | 82.556 | 4.452 | 8.859 | 1.00 | 37.55 |
| ATOM | 2300 | C | LEU | 473 | 85.283 | 7.623 | 9.601 | 1.00 | 38.21 |
| ATOM | 2301 | O | LEU | 473 | 84.696 | 8.631 | 9.187 | 1.00 | 38.52 |
| ATOM | 2302 | N | PRO | 474 | 86.412 | 7.156 | 9.025 | 1.00 | 37.74 |
| ATOM | 2303 | CD | PRO | 474 | 87.292 | 6.107 | 9.568 | 1.00 | 36.38 |
| ATOM | 2304 | CA | PRO | 474 | 87.010 | 7.753 | 7.824 | 1.00 | 36.91 |
| ATOM | 2305 | CB | PRO | 474 | 88.233 | 6.865 | 7.587 | 1.00 | 34.65 |
| ATOM | 2306 | CG | PRO | 474 | 88.620 | 6.477 | 8.967 | 1.00 | 32.99 |
| ATOM | 2307 | C | PRO | 474 | 86.036 | 7.663 | 6.660 | 1.00 | 38.15 |
| ATOM | 2308 | O | PRO | 474 | 85.536 | 6.578 | 6.362 | 1.00 | 38.24 |
| ATOM | 2309 | N | ARG | 475 | 85.793 | 8.784 | 5.981 | 1.00 | 38.90 |
| ATOM | 2310 | CA | ARG | 475 | 84.846 | 8.802 | 4.863 | 1.00 | 41.23 |
| ATOM | 2311 | CB | ARG | 475 | 84.743 | 10.206 | 4.258 | 1.00 | 38.36 |
| ATOM | 2312 | CG | ARG | 475 | 84.311 | 11.271 | 5.267 | 1.00 | 35.30 |
| ATOM | 2313 | CD | ARG | 475 | 84.282 | 12.691 | 4.679 | 1.00 | 35.23 |
| ATOM | 2314 | NE | ARG | 475 | 83.850 | 13.658 | 5.679 | 1.00 | 27.27 |
| ATOM | 2315 | CZ | ARG | 475 | 82.585 | 13.859 | 6.011 | 1.00 | 25.77 |
| ATOM | 2316 | NH1 | ARG | 475 | 81.630 | 13.181 | 5.402 | 1.00 | 25.09 |
| ATOM | 2317 | NH2 | ARG | 475 | 82.286 | 14.639 | 7.047 | 1.00 | 25.24 |
| ATOM | 2318 | C | ARG | 475 | 85.101 | 7.745 | 3.791 | 1.00 | 42.43 |
| ATOM | 2319 | O | ARG | 475 | 84.160 | 7.212 | 3.204 | 1.00 | 44.06 |
| ATOM | 2320 | N | ASP | 476 | 86.359 | 7.381 | 3.594 | 1.00 | 44.69 |
| ATOM | 2321 | CA | ASP | 476 | 86.690 | 6.384 | 2.583 | 1.00 | 48.37 |
| ATOM | 2322 | CB | ASP | 476 | 88.197 | 6.371 | 2.319 | 1.00 | 52.12 |
| ATOM | 2323 | CG | ASP | 476 | 88.988 | 5.925 | 3.521 | 1.00 | 56.56 |
| ATOM | 2324 | OD1 | ASP | 476 | 89.299 | 4.718 | 3.613 | 1.00 | 59.72 |
| ATOM | 2325 | OD2 | ASP | 476 | 89.294 | 6.779 | 4.376 | 1.00 | 61.19 |
| ATOM | 2326 | C | ASP | 476 | 86.210 | 4.988 | 2.973 | 1.00 | 49.50 |
| ATOM | 2327 | O | ASP | 476 | 86.204 | 4.074 | 2.145 | 1.00 | 51.61 |
| ATOM | 2328 | N | ARG | 477 | 85.852 | 4.814 | 4.241 | 1.00 | 48.26 |
| ATOM | 2329 | CA | ARG | 477 | 85.357 | 3.525 | 4.732 | 1.00 | 47.16 |
| ATOM | 2330 | CB | ARG | 477 | 85.909 | 3.252 | 6.126 | 1.00 | 49.76 |
| ATOM | 2331 | CG | ARG | 477 | 87.325 | 2.723 | 6.088 | 1.00 | 53.26 |
| ATOM | 2332 | CD | ARG | 477 | 88.043 | 2.898 | 7.406 | 1.00 | 58.02 |
| ATOM | 2333 | NE | ARG | 477 | 87.394 | 2.213 | 8.517 | 1.00 | 61.16 |
| ATOM | 2334 | CZ | ARG | 477 | 87.810 | 2.297 | 9.776 | 1.00 | 63.35 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2335 | NH1 | ARG | 477 | 88.875 | 3.032 | 10.081 | 1.00 | 64.92 |
| ATOM | 2336 | NH2 | ARG | 477 | 87.139 | 1.675 | 10.738 | 1.00 | 66.00 |
| ATOM | 2337 | C | ARG | 477 | 83.822 | 3.445 | 4.740 | 1.00 | 45.38 |
| ATOM | 2338 | O | ARG | 477 | 83.239 | 2.540 | 5.336 | 1.00 | 43.67 |
| ATOM | 2339 | N | LEU | 478 | 83.175 | 4.364 | 4.026 | 1.00 | 42.09 |
| ATOM | 2340 | CA | LEU | 478 | 81.721 | 4.410 | 3.951 | 1.00 | 37.74 |
| ATOM | 2341 | CB | LEU | 478 | 81.198 | 5.539 | 4.849 | 1.00 | 32.19 |
| ATOM | 2342 | CG | LEU | 478 | 79.673 | 5.638 | 4.973 | 1.00 | 30.21 |
| ATOM | 2343 | CD1 | LEU | 478 | 79.146 | 4.635 | 5.983 | 1.00 | 22.82 |
| ATOM | 2344 | CD2 | LEU | 478 | 79.313 | 7.035 | 5.422 | 1.00 | 34.82 |
| ATOM | 2345 | C | LEU | 478 | 81.329 | 4.702 | 2.514 | 1.00 | 38.75 |
| ATOM | 2346 | O | LEU | 478 | 81.818 | 5.669 | 1.935 | 1.00 | 40.60 |
| ATOM | 2347 | N | VAL | 479 | 80.477 | 3.863 | 1.925 | 1.00 | 38.78 |
| ATOM | 2348 | CA | VAL | 479 | 80.020 | 4.058 | 0.544 | 1.00 | 37.97 |
| ATOM | 2349 | CB | VAL | 479 | 80.353 | 2.845 | -0.360 | 1.00 | 36.36 |
| ATOM | 2350 | CG1 | VAL | 479 | 79.837 | 3.090 | -1.759 | 1.00 | 33.55 |
| ATOM | 2351 | CG2 | VAL | 479 | 81.868 | 2.626 | -0.405 | 1.00 | 33.76 |
| ATOM | 2352 | C | VAL | 479 | 78.523 | 4.298 | 0.562 | 1.00 | 37.83 |
| ATOM | 2353 | O | VAL | 479 | 77.750 | 3.383 | 0.820 | 1.00 | 37.70 |
| ATOM | 2354 | N | LEU | 480 | 78.127 | 5.542 | 0.305 | 1.00 | 39.32 |
| ATOM | 2355 | CA | LEU | 480 | 76.723 | 5.942 | 0.333 | 1.00 | 38.41 |
| ATOM | 2356 | CB | LEU | 480 | 76.630 | 7.458 | 0.224 | 1.00 | 38.29 |
| ATOM | 2357 | CG | LEU | 480 | 77.287 | 8.226 | 1.377 | 1.00 | 37.99 |
| ATOM | 2358 | CD1 | LEU | 480 | 77.098 | 9.730 | 1.159 | 1.00 | 34.00 |
| ATOM | 2359 | CD2 | LEU | 480 | 76.666 | 7.785 | 2.703 | 1.00 | 32.79 |
| ATOM | 2360 | C | LEU | 480 | 75.893 | 5.287 | -0.753 | 1.00 | 38.24 |
| ATOM | 2361 | O | LEU | 480 | 76.315 | 5.205 | -1.903 | 1.00 | 39.11 |
| ATOM | 2362 | N | GLY | 481 | 74.672 | 4.896 | -0.394 | 1.00 | 36.70 |
| ATOM | 2363 | CA | GLY | 481 | 73.811 | 4.223 | -1.357 | 1.00 | 36.53 |
| ATOM | 2364 | C | GLY | 481 | 72.417 | 4.782 | -1.524 | 1.00 | 37.61 |
| ATOM | 2365 | O | GLY | 481 | 72.159 | 5.961 | -1.277 | 1.00 | 40.02 |
| ATOM | 2366 | N | LYS | 482 | 71.484 | 3.913 | -1.911 | 1.00 | 37.52 |
| ATOM | 2367 | CA | LYS | 482 | 70.099 | 4.313 | -2.153 | 1.00 | 39.89 |
| ATOM | 2368 | CB | LYS | 482 | 69.243 | 3.104 | -2.551 | 1.00 | 42.44 |
| ATOM | 2369 | C | LYS | 482 | 69.447 | 5.028 | -0.984 | 1.00 | 41.25 |
| ATOM | 2370 | O | LYS | 482 | 69.538 | 4.589 | 0.163 | 1.00 | 42.22 |
| ATOM | 2371 | N | PRO | 483 | 68.779 | 6.156 | -1.263 | 1.00 | 41.71 |
| ATOM | 2372 | CD | PRO | 483 | 68.643 | 6.876 | -2.537 | 1.00 | 41.01 |
| ATOM | 2373 | CA | PRO | 483 | 68.118 | 6.889 | -0.193 | 1.00 | 42.72 |
| ATOM | 2374 | CB | PRO | 483 | 67.606 | 8.146 | -0.906 | 1.00 | 41.26 |
| ATOM | 2375 | CG | PRO | 483 | 67.425 | 7.713 | -2.290 | 1.00 | 40.16 |
| ATOM | 2376 | C | PRO | 483 | 66.999 | 6.061 | 0.429 | 1.00 | 44.69 |
| ATOM | 2377 | O | PRO | 483 | 66.306 | 5.314 | -0.262 | 1.00 | 45.26 |
| ATOM | 2378 | N | LEU | 484 | 66.883 | 6.163 | 1.751 | 1.00 | 45.34 |
| ATOM | 2379 | CA | LEU | 484 | 65.872 | 5.450 | 2 512 | 1.00 | 47.34 |
| ATOM | 2380 | CB | LEU | 484 | 66.494 | 4.793 | 3.746 | 1.00 | 42.40 |
| ATOM | 2381 | CG | LEU | 484 | 67.517 | 3.668 | 3.535 | 1.00 | 39.50 |
| ATOM | 2382 | CD1 | LEU | 484 | 68.208 | 3.337 | 4.828 | 1.00 | 33.64 |
| ATOM | 2383 | CD2 | LEU | 484 | 66.861 | 2.419 | 3.003 | 1.00 | 33.44 |
| ATOM | 2384 | C | LEU | 484 | 64.733 | 6.391 | 2.927 | 1.00 | 52.14 |
| ATOM | 2385 | O | LEU | 484 | 63.611 | 5.941 | 3.142 | 1.00 | 53.64 |
| ATOM | 2386 | N | GLY | 485 | 65.013 | 7.697 | 3.025 | 1.00 | 55.25 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2387 | CA | GLY | 485 | 63.982 | 8.653 | 3.427 | 1.00 | 58.76 |
| ATOM | 2388 | C | GLY | 485 | 64.441 | 10.104 | 3.503 | 1.00 | 60.58 |
| ATOM | 2389 | O | GLY | 485 | 65.640 | 10.376 | 3.600 | 1.00 | 61.49 |
| ATOM | 2390 | N | ALA | 486 | 63.490 | 11.032 | 3.489 | 1.00 | 61.46 |
| ATOM | 2391 | CA | ALA | 486 | 63.791 | 12.458 | 3.545 | 1.00 | 63.24 |
| ATOM | 2392 | CB | ALA | 486 | 63.847 | 13.035 | 2.126 | 1.00 | 64.42 |
| ATOM | 2393 | C | ALA | 486 | 62.730 | 13.179 | 4.355 | 1.00 | 63.86 |
| ATOM | 2394 | O | ALA | 486 | 61.655 | 12.633 | 4.599 | 1.00 | 65.24 |
| ATOM | 2395 | N | GLY | 487 | 63.022 | 14.404 | 4.768 | 1.00 | 63.89 |
| ATOM | 2396 | CA | GLY | 487 | 62.054 | 15.158 | 5.538 | 1.00 | 64.30 |
| ATOM | 2397 | C | GLY | 487 | 62.431 | 16.617 | 5.623 | 1.00 | 65.34 |
| ATOM | 2398 | O | GLY | 487 | 63.071 | 17.154 | 4.718 | 1.00 | 65.98 |
| ATOM | 2399 | N | ALA | 488 | 62.023 | 17.259 | 6.711 | 1.00 | 66.16 |
| ATOM | 2400 | CA | ALA | 488 | 62.317 | 18.666 | 6.934 | 1.00 | 66.71 |
| ATOM | 2401 | CB | ALA | 488 | 61.647 | 19.132 | 8.219 | 1.00 | 70.05 |
| ATOM | 2402 | C | ALA | 488 | 63.828 | 18.844 | 7.027 | 1.00 | 66.55 |
| ATOM | 2403 | O | ALA | 488 | 64.432 | 18.547 | 8.063 | 1.00 | 65.59 |
| ATOM | 2404 | N | PHE | 489 | 64.430 | 19.228 | 5.904 | 1.00 | 65.54 |
| ATOM | 2405 | CA | PHE | 489 | 65.875 | 19.457 | 5.807 | 1.00 | 65.40 |
| ATOM | 2406 | CB | PHE | 489 | 66.244 | 20.775 | 6.498 | 1.00 | 67.06 |
| ATOM | 2407 | C | PHE | 489 | 66.773 | 18.296 | 6.311 | 1.00 | 64.01 |
| ATOM | 2408 | O | PHE | 489 | 67.942 | 18.502 | 6.651 | 1.00 | 62.51 |
| ATOM | 2409 | N | GLY | 490 | 66.234 | 17.075 | 6.288 | 1.00 | 61.41 |
| ATOM | 2410 | CA | GLY | 490 | 66.974 | 15.901 | 6.724 | 1.00 | 55.89 |
| ATOM | 2411 | C | GLY | 490 | 66.858 | 14.821 | 5.667 | 1.00 | 53.58 |
| ATOM | 2412 | O | GLY | 490 | 65.825 | 14.703 | 5.000 | 1.00 | 54.22 |
| ATOM | 2413 | N | GLN | 491 | 67.899 | 14.006 | 5.543 | 1.00 | 51.23 |
| ATOM | 2414 | CA | GLN | 491 | 67.966 | 12.934 | 4.556 | 1.00 | 47.90 |
| ATOM | 2415 | CB | GLN | 491 | 68.823 | 13.445 | 3.387 | 1.00 | 50.09 |
| ATOM | 2416 | CG | GLN | 491 | 68.979 | 12.529 | 2.183 | 1.00 | 56.77 |
| ATOM | 2417 | CD | GLN | 491 | 69.945 | 13.115 | 1.161 | 1.00 | 60.83 |
| ATOM | 2418 | OE1 | GLN | 491 | 70.283 | 14.292 | 1.218 | 1.00 | 65.11 |
| ATOM | 2419 | NE2 | GLN | 491 | 70.411 | 12.284 | 0.232 | 1.00 | 63.81 |
| ATOM | 2420 | C | GLN | 491 | 68.597 | 11.673 | 5.190 | 1.00 | 45.27 |
| ATOM | 2421 | O | GLN | 491 | 69.507 | 11.758 | 6.014 | 1.00 | 45.41 |
| ATOM | 2422 | N | VAL | 492 | 68.112 | 10.503 | 4.805 | 1.00 | 41.69 |
| ATOM | 2423 | CA | VAL | 492 | 68.624 | 9.245 | 5.325 | 1.00 | 39.95 |
| ATOM | 2424 | CB | VAL | 492 | 67.583 | 8.528 | 6.230 | 1.00 | 41.77 |
| ATOM | 2425 | CG1 | VAL | 492 | 68.117 | 7.168 | 6.701 | 1.00 | 39.86 |
| ATOM | 2426 | CG2 | VAL | 492 | 67.226 | 9.399 | 7.421 | 1.00 | 42.87 |
| ATOM | 2427 | C | VAL | 492 | 68.911 | 8.348 | 4.126 | 1.00 | 38.86 |
| ATOM | 2428 | O | VAL | 492 | 68.025 | 8.114 | 3.301 | 1.00 | 37.55 |
| ATOM | 2429 | N | VAL | 493 | 70.141 | 7.862 | 4.010 | 1.00 | 36.01 |
| ATOM | 2430 | CA | VAL | 493 | 70.481 | 6.994 | 2.895 | 1.00 | 37.55 |
| ATOM | 2431 | CB | VAL | 493 | 71.471 | 7.674 | 1.889 | 1.00 | 38.65 |
| ATOM | 2432 | CG1 | VAL | 493 | 71.128 | 9.137 | 1.709 | 1.00 | 37.08 |
| ATOM | 2433 | CG2 | VAL | 493 | 72.929 | 7.498 | 2.318 | 1.00 | 39.03 |
| ATOM | 2434 | C | VAL | 493 | 71.071 | 5.678 | 3.371 | 1.00 | 38.61 |
| ATOM | 2435 | O | VAL | 493 | 71.645 | 5.599 | 4.456 | 1.00 | 39.75 |
| ATOM | 2436 | N | LEU | 494 | 70.899 | 4.637 | 2.572 | 1.00 | 39.68 |
| ATOM | 2437 | CA | LEU | 494 | 71.460 | 3.345 | 2.910 | 1.00 | 40.98 |
| ATOM | 2438 | CB | LEU | 494 | 70.748 | 2.241 | 2.123 | 1.00 | 42.14 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2439 | CG | LEU | 494 | 71.250 | 0.808 | 2.305 | 1.00 | 40.33 |
| ATOM | 2440 | CD1 | LEU | 494 | 71.186 | 0.425 | 3.765 | 1.00 | 39.62 |
| ATOM | 2441 | CD2 | LEU | 494 | 70.411 | -0.117 | 1.459 | 1.00 | 40.75 |
| ATOM | 2442 | C | LEU | 494 | 72.918 | 3.432 | 2.483 | 1.00 | 40.66 |
| ATOM | 2443 | O | LEU | 494 | 73.249 | 4.163 | 1.552 | 1.00 | 40.05 |
| ATOM | 2444 | N | ALA | 495 | 73.798 | 2.725 | 3.169 | 1.00 | 39.74 |
| ATOM | 2445 | CA | ALA | 495 | 75.202 | 2.768 | 2.820 | 1.00 | 42.06 |
| ATOM | 2446 | CB | ALA | 495 | 75.858 | 3.999 | 3.468 | 1.00 | 42.91 |
| ATOM | 2447 | C | ALA | 495 | 75.887 | 1.497 | 3.289 | 1.00 | 43.34 |
| ATOM | 2448 | O | ALA | 495 | 75.271 | 0.668 | 3.946 | 1.00 | 43.81 |
| ATOM | 2449 | N | GLU | 496 | 77.140 | 1.314 | 2.880 | 1.00 | 44.40 |
| ATOM | 2450 | CA | GLU | 496 | 77.910 | 0.154 | 3.297 | 1.00 | 45.12 |
| ATOM | 2451 | CB | GLU | 496 | 78.282 | -0.722 | 2.106 | 1.00 | 48.62 |
| ATOM | 2452 | CG | GLU | 496 | 77.062 | -1.206 | 1.346 | 1.00 | 56.98 |
| ATOM | 2453 | CD | GLU | 496 | 77.316 | -2.476 | 0.567 | 1.00 | 60.32 |
| ATOM | 2454 | OE1 | GLU | 496 | 76.448 | -3.378 | 0.634 | 1.00 | 62.17 |
| ATOM | 2455 | OE2 | GLU | 496 | 78.371 | -2.575 | -0.103 | 1.00 | 60.48 |
| ATOM | 2456 | C | GLU | 496 | 79.151 | 0.658 | 3.987 | 1.00 | 43.27 |
| ATOM | 2457 | O | GLU | 496 | 79.957 | 1.366 | 3.387 | 1.00 | 44.49 |
| ATOM | 2458 | N | ALA | 497 | 79.232 | 0.385 | 5.282 | 1.00 | 43.29 |
| ATOM | 2459 | CA | ALA | 497 | 80.374 | 0.799 | 6.086 | 1.00 | 44.01 |
| ATOM | 2460 | CB | ALA | 497 | 79.910 | 1.182 | 7.471 | 1.00 | 42.35 |
| ATOM | 2461 | C | ALA | 497 | 81.381 | -0.351 | 6.150 | 1.00 | 45.60 |
| ATOM | 2462 | O | ALA | 497 | 80.997 | -1.512 | 6.107 | 1.00 | 43.35 |
| ATOM | 2463 | N | ILE | 498 | 82.666 | -0.025 | 6.206 | 1.00 | 48.78 |
| ATOM | 2464 | CA | ILE | 498 | 83.709 | -1.042 | 6.262 | 1.00 | 49.43 |
| ATOM | 2465 | CB | ILE | 498 | 84.611 | -0.977 | 5.014 | 1.00 | 50.66 |
| ATOM | 2466 | CG2 | ILE | 498 | 85.681 | -2.054 | 5.082 | 1.00 | 51.85 |
| ATOM | 2467 | CG1 | ILE | 498 | 83.780 | -1.150 | 3.741 | 1.00 | 50.27 |
| ATOM | 2468 | CD1 | ILE | 498 | 83.073 | 0.112 | 3.255 | 1.00 | 54.24 |
| ATOM | 2469 | C | ILE | 498 | 84.572 | -0.878 | 7.510 | 1.00 | 50.32 |
| ATOM | 2470 | O | ILE | 498 | 85.055 | 0.219 | 7.801 | 1.00 | 49.08 |
| ATOM | 2471 | N | GLY | 499 | 84.713 | -1.964 | 8.270 | 1.00 | 51.88 |
| ATOM | 2472 | CA | GLY | 499 | 85.526 | -1.958 | 9.480 | 1.00 | 55.86 |
| ATOM | 2473 | C | GLY | 499 | 85.061 | -1.111 | 10.661 | 1.00 | 59.72 |
| ATOM | 2474 | O | GLY | 499 | 85.885 | -0.545 | 11.393 | 1.00 | 61.66 |
| ATOM | 2475 | N | LEU | 500 | 83.747 | -1.058 | 10.878 | 1.00 | 59.88 |
| ATOM | 2476 | CA | LEU | 500 | 83.167 | -0.275 | 11.974 | 1.00 | 58.62 |
| ATOM | 2477 | CB | LEU | 500 | 81.663 | -0.556 | 12.086 | 1.00 | 57.41 |
| ATOM | 2478 | CG | LEU | 500 | 80.764 | -0.090 | 10.937 | 1.00 | 55.24 |
| ATOM | 2479 | CD1 | LEU | 500 | 79.331 | -0.536 | 11.168 | 1.00 | 51.91 |
| ATOM | 2480 | CD2 | LEU | 500 | 80.845 | 1.426 | 10.799 | 1.00 | 54.93 |
| ATOM | 2481 | C | LEU | 500 | 83.849 | -0.565 | 13.306 | 1.00 | 58.51 |
| ATOM | 2482 | O | LEU | 500 | 84.226 | -1.710 | 13.576 | 1.00 | 60.71 |
| ATOM | 2483 | N | PRO | 505 | 87.501 | -6.102 | 10.460 | 1.00 | 82.25 |
| ATOM | 2484 | CD | PRO | 505 | 88.578 | -6.722 | 11.248 | 1.00 | 82.69 |
| ATOM | 2485 | CA | PRO | 505 | 87.860 | -4.730 | 10.077 | 1.00 | 80.47 |
| ATOM | 2486 | CB | PRO | 505 | 89.257 | -4.557 | 10.686 | 1.00 | 80.88 |
| ATOM | 2487 | CG | PRO | 505 | 89.782 | -5.960 | 10.770 | 1.00 | 81.84 |
| ATOM | 2488 | C | PRO | 505 | 87.850 | -4.508 | 8.567 | 1.00 | 77.40 |
| ATOM | 2489 | O | PRO | 505 | 88.038 | -3.391 | 8.087 | 1.00 | 76.83 |
| ATOM | 2490 | N | ASN | 506 | 87.632 | -5.584 | 7.826 | 1.00 | 74.91 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2491 | CA | ASN | 506 | 87.572 | -5.502 | 6.375 | 1.00 | 73.04 |
| ATOM | 2492 | CB | ASN | 506 | 88.632 | -6.406 | 5.749 | 1.00 | 73.39 |
| ATOM | 2493 | C | ASN | 506 | 86.180 | -5.938 | 5.929 | 1.00 | 71.75 |
| ATOM | 2494 | O | ASN | 506 | 85.918 | -6.094 | 4.739 | 1.00 | 71.33 |
| ATOM | 2495 | N | ARG | 507 | 85.294 | -6.124 | 6.905 | 1.00 | 69.66 |
| ATOM | 2496 | CA | ARG | 507 | 83.924 | -6.534 | 6.638 | 1.00 | 66.59 |
| ATOM | 2497 | CB | ARG | 507 | 83.369 | -7.329 | 7.819 | 1.00 | 69.86 |
| ATOM | 2498 | C | ARG | 507 | 83.048 | -5.321 | 6.409 | 1.00 | 63.59 |
| ATOM | 2499 | O | ARG | 507 | 83.225 | -4.291 | 7.070 | 1.00 | 64.09 |
| ATOM | 2500 | N | VAL | 508 | 82.126 | -5.429 | 5.462 | 1.00 | 59.52 |
| ATOM | 2501 | CA | VAL | 508 | 81.217 | -4.334 | 5.187 | 1.00 | 57.28 |
| ATOM | 2502 | CB | VAL | 508 | 80.905 | -4.178 | 3.686 | 1.00 | 55.73 |
| ATOM | 2503 | CG1 | VAL | 508 | 82.163 | -3.952 | 2.922 | 1.00 | 57.01 |
| ATOM | 2504 | CG2 | VAL | 508 | 80.184 | -5.390 | 3.149 | 1.00 | 58.06 |
| ATOM | 2505 | C | VAL | 508 | 79.928 | -4.614 | 5.935 | 1.00 | 57.10 |
| ATOM | 2506 | O | VAL | 508 | 79.483 | -5.759 | 6.018 | 1.00 | 57.35 |
| ATOM | 2507 | N | THR | 509 | 79.345 | -3.555 | 6.482 | 1.00 | 55.31 |
| ATOM | 2508 | CA | THR | 509 | 78.107 | -3.652 | 7.227 | 1.00 | 50.14 |
| ATOM | 2509 | CB | THR | 509 | 78.329 | -3.192 | 8.686 | 1.00 | 50.91 |
| ATOM | 2510 | OG1 | THR | 509 | 79.476 | -3.851 | 9.227 | 1.00 | 49.20 |
| ATOM | 2511 | CG2 | THR | 509 | 77.123 | -3.524 | 9.559 | 1.00 | 51.96 |
| ATOM | 2512 | C | THR | 509 | 77.140 | -2.705 | 6.528 | 1.00 | 47.53 |
| ATOM | 2513 | O | THR | 509 | 77.485 | -1.558 | 6.242 | 1.00 | 47.22 |
| ATOM | 2514 | N | LYS | 510 | 75.958 | -3.191 | 6.191 | 1.00 | 45.64 |
| ATOM | 2515 | CA | LYS | 510 | 74.975 | -2.333 | 5.551 | 1.00 | 44.44 |
| ATOM | 2516 | CB | LYS | 510 | 73.861 | -3.175 | 4.948 | 1.00 | 46.74 |
| ATOM | 2517 | CG | LYS | 510 | 73.008 | -2.420 | 3.950 | 1.00 | 54.51 |
| ATOM | 2518 | CD | LYS | 510 | 73.463 | -2.645 | 2.513 | 1.00 | 54.97 |
| ATOM | 2519 | CE | LYS | 510 | 72.846 | -3.917 | 1.934 | 1.00 | 58.25 |
| ATOM | 2520 | NZ | LYS | 510 | 73.112 | -5.150 | 2.740 | 1.00 | 58.33 |
| ATOM | 2521 | C | LYS | 510 | 74.430 | -1.470 | 6.696 | 1.00 | 42.75 |
| ATOM | 2522 | O | LYS | 510 | 74.053 | -2.006 | 7.742 | 1.00 | 43.14 |
| ATOM | 2523 | N | VAL | 511 | 74.443 | -0.149 | 6.531 | 1.00 | 38.63 |
| ATOM | 2524 | CA | VAL | 511 | 73.975 | 0.757 | 7.576 | 1.00 | 34.16 |
| ATOM | 2525 | CB | VAL | 511 | 75.161 | 1.399 | 8.333 | 1.00 | 35.66 |
| ATOM | 2526 | CG1 | VAL | 511 | 75.922 | 0.340 | 9.100 | 1.00 | 31.46 |
| ATOM | 2527 | CG2 | VAL | 511 | 76.098 | 2.100 | 7.357 | 1.00 | 35.08 |
| ATOM | 2528 | C | VAL | 511 | 73.116 | 1.873 | 7.024 | 1.00 | 31.58 |
| ATOM | 2529 | O | VAL | 511 | 72.962 | 1.984 | 5.818 | 1.00 | 33.18 |
| ATOM | 2530 | N | ALA | 512 | 72.542 | 2.687 | 7.906 | 1.00 | 30.77 |
| ATOM | 2531 | CA | ALA | 512 | 71.724 | 3.818 | 7.484 | 1.00 | 28.58 |
| ATOM | 2532 | CB | ALA | 512 | 70.382 | 3.774 | 8.145 | 1.00 | 26.09 |
| ATOM | 2533 | C | ALA | 512 | 72.487 | 5.075 | 7.905 | 1.00 | 29.94 |
| ATOM | 2534 | O | ALA | 512 | 72.996 | 5.151 | 9.031 | 1.00 | 29.90 |
| ATOM | 2535 | N | VAL | 513 | 72.556 | 6.057 | 7.012 | 1.00 | 28.68 |
| ATOM | 2536 | CA | VAL | 513 | 73.286 | 7.290 | 7.280 | 1.00 | 28.26 |
| ATOM | 2537 | CB | VAL | 513 | 74.439 | 7.503 | 6.269 | 1.00 | 26.92 |
| ATOM | 2538 | CG1 | VAL | 513 | 75.213 | 8.730 | 6.618 | 1.00 | 25.26 |
| ATOM | 2539 | CG2 | VAL | 513 | 75.353 | 6.308 | 6.238 | 1.00 | 25.10 |
| ATOM | 2540 | C | VAL | 513 | 72.383 | 8.526 | 7.230 | 1.00 | 29.54 |
| ATOM | 2541 | O | VAL | 513 | 71.745 | 8.799 | 6.200 | 1.00 | 28.56 |
| ATOM | 2542 | N | LYS | 514 | 72.304 | 9.228 | 8.359 | 1.00 | 28.94 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2543 | CA | LYS | 514 | 71.519 | 10.450 | 8.481 | 1.00 | 28.60 |
| ATOM | 2544 | CB | LYS | 514 | 70.942 | 10.611 | 9.893 | 1.00 | 31.19 |
| ATOM | 2545 | CG | LYS | 514 | 69.988 | 9.542 | 10.328 | 1.00 | 31.41 |
| ATOM | 2546 | CD | LYS | 514 | 69.454 | 9.922 | 11.690 | 1.00 | 40.14 |
| ATOM | 2547 | CE | LYS | 514 | 68.484 | 8.892 | 12.222 | 1.00 | 48.93 |
| ATOM | 2548 | NZ | LYS | 514 | 67.198 | 8.861 | 11.475 | 1.00 | 57.07 |
| ATOM | 2549 | C | LYS | 514 | 72.430 | 11.636 | 8.196 | 1.00 | 25.53 |
| ATOM | 2550 | O | LYS | 514 | 73.544 | 11.714 | 8.722 | 1.00 | 20.42 |
| ATOM | 2551 | N | MET | 515 | 71.928 | 12.576 | 7.407 | 1.00 | 26.63 |
| ATOM | 2552 | CA | MET | 515 | 72.676 | 13.762 | 7.008 | 1.00 | 27.59 |
| ATOM | 2553 | CB | MET | 515 | 73.425 | 13.487 | 5.693 | 1.00 | 28.22 |
| ATOM | 2554 | CG | MET | 515 | 72.502 | 13.026 | 4.556 | 1.00 | 28.70 |
| ATOM | 2555 | SD | MET | 515 | 73.377 | 12.418 | 3.113 | 1.00 | 32.30 |
| ATOM | 2556 | CE | MET | 515 | 73.949 | 10.803 | 3.715 | 1.00 | 24.88 |
| ATOM | 2557 | C | MET | 515 | 71.683 | 14.880 | 6.779 | 1.00 | 28.41 |
| ATOM | 2558 | O | MET | 515 | 70.472 | 14.685 | 6.889 | 1.00 | 32.15 |
| ATOM | 2559 | N | LEU | 516 | 72.202 | 16.056 | 6.466 | 1.00 | 29.12 |
| ATOM | 2560 | CA | LEU | 516 | 71.383 | 17.220 | 6.180 | 1.00 | 29.98 |
| ATOM | 2561 | CB | LEU | 516 | 72.110 | 18.512 | 6.593 | 1.00 | 25.32 |
| ATOM | 2562 | CG | LEU | 516 | 72.455 | 18.767 | 8.067 | 1.00 | 26.60 |
| ATOM | 2563 | CD1 | LEU | 516 | 73.210 | 20.057 | 8.190 | 1.00 | 24.56 |
| ATOM | 2564 | CD2 | LEU | 516 | 71.217 | 18.844 | 8.900 | 1.00 | 22.75 |
| ATOM | 2565 | C | LEU | 516 | 71.092 | 17.274 | 4.674 | 1.00 | 31.50 |
| ATOM | 2566 | O | LEU | 516 | 71.763 | 16.636 | 3.873 | 1.00 | 32.97 |
| ATOM | 2567 | N | LYS | 517 | 70.069 | 18.018 | 4.293 | 1.00 | 33.29 |
| ATOM | 2568 | CA | LYS | 517 | 69.755 | 18.187 | 2.890 | 1.00 | 32.20 |
| ATOM | 2569 | CB | LYS | 517 | 68.246 | 18.363 | 2.699 | 1.00 | 36.34 |
| ATOM | 2570 | CG | LYS | 517 | 67.432 | 17.182 | 3.192 | 1.00 | 43.49 |
| ATOM | 2571 | CD | LYS | 517 | 66.172 | 16.940 | 2.356 | 1.00 | 53.91 |
| ATOM | 2572 | CE | LYS | 517 | 65.088 | 17.984 | 2.581 | 1.00 | 58.71 |
| ATOM | 2573 | NZ | LYS | 517 | 63.902 | 17.740 | 1.704 | 1.00 | 59.37 |
| ATOM | 2574 | C | LYS | 517 | 70.520 | 19.455 | 2.507 | 1.00 | 31.31 |
| ATOM | 2575 | O | LYS | 517 | 70.917 | 20.217 | 3.383 | 1.00 | 28.74 |
| ATOM | 2576 | N | SER | 518 | 70.744 | 19.672 | 1.213 | 1.00 | 32.48 |
| ATOM | 2577 | CA | SER | 518 | 71.486 | 20.840 | 0.714 | 1.00 | 33.52 |
| ATOM | 2578 | CB | SER | 518 | 71.611 | 20.772 | -0.809 | 1.00 | 32.98 |
| ATOM | 2579 | OG | SER | 518 | 70.375 | 20.407 | -1.396 | 1.00 | 36.75 |
| ATOM | 2580 | C | SER | 518 | 70.896 | 22.189 | 1.110 | 1.00 | 34.62 |
| ATOM | 2581 | O | SER | 518 | 71.580 | 23.214 | 1.058 | 1.00 | 34.57 |
| ATOM | 2582 | N | ASP | 519 | 69.624 | 22.193 | 1.485 | 1.00 | 35.47 |
| ATOM | 2583 | CA | ASP | 519 | 68.943 | 23.422 | 1.885 | 1.00 | 36.10 |
| ATOM | 2584 | CB | ASP | 519 | 67.529 | 23.480 | 1.268 | 1.00 | 38.11 |
| ATOM | 2585 | CG | ASP | 519 | 66.668 | 22.258 | 1.608 | 1.00 | 41.64 |
| ATOM | 2586 | OD1 | ASP | 519 | 67.150 | 21.309 | 2.253 | 1.00 | 41.70 |
| ATOM | 2587 | OD2 | ASP | 519 | 65.478 | 22.250 | 1.220 | 1.00 | 49.25 |
| ATOM | 2588 | C | ASP | 519 | 68.881 | 23.645 | 3.395 | 1.00 | 34.66 |
| ATOM | 2589 | O | ASP | 519 | 68.266 | 24.602 | 3.860 | 1.00 | 33.39 |
| ATOM | 2590 | N | ALA | 520 | 69.551 | 22.784 | 4.150 | 1.00 | 33.52 |
| ATOM | 2591 | CA | ALA | 520 | 69.561 | 22.895 | 5.605 | 1.00 | 32.12 |
| ATOM | 2592 | CB | ALA | 520 | 70.253 | 21.687 | 6.207 | 1.00 | 32.08 |
| ATOM | 2593 | C | ALA | 520 | 70.242 | 24.163 | 6.076 | 1.00 | 30.91 |
| ATOM | 2594 | O | ALA | 520 | 71.014 | 24.778 | 5.331 | 1.00 | 30.57 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2595 | N | THR | 521 | 69.943 | 24.555 | 7.311 | 1.00 | 30.80 |
| ATOM | 2596 | CA | THR | 521 | 70.546 | 25.738 | 7.921 | 1.00 | 32.33 |
| ATOM | 2597 | CB | THR | 521 | 69.493 | 26.763 | 8.440 | 1.00 | 34.30 |
| ATOM | 2598 | OG1 | THR | 521 | 68.817 | 26.242 | 9.598 | 1.00 | 35.14 |
| ATOM | 2599 | CG2 | THR | 521 | 68.484 | 27.109 | 7.366 | 1.00 | 37.70 |
| ATOM | 2600 | C | THR | 521 | 71.418 | 25.312 | 9.098 | 1.00 | 33.11 |
| ATOM | 2601 | O | THR | 521 | 71.518 | 24.125 | 9.426 | 1.00 | 31.39 |
| ATOM | 2602 | N | GLU | 522 | 72.022 | 26.293 | 9.753 | 1.00 | 34.91 |
| ATOM | 2603 | CA | GLU | 522 | 72.882 | 26.048 | 10.901 | 1.00 | 39.44 |
| ATOM | 2604 | CB | GLU | 522 | 73.516 | 27.357 | 11.360 | 1.00 | 46.96 |
| ATOM | 2605 | CG | GLU | 522 | 74.550 | 27.220 | 12.488 | 1.00 | 59.20 |
| ATOM | 2606 | CD | GLU | 522 | 75.919 | 26.740 | 12.011 | 1.00 | 64.70 |
| ATOM | 2607 | OE1 | GLU | 522 | 76.910 | 27.478 | 12.219 | 1.00 | 63.87 |
| ATOM | 2608 | OE2 | GLU | 522 | 76.006 | 25.627 | 11.445 | 1.00 | 71.55 |
| ATOM | 2609 | C | GLU | 522 | 72.083 | 25.428 | 12.044 | 1.00 | 39.61 |
| ATOM | 2610 | O | GLU | 522 | 72.587 | 24.554 | 12.757 | 1.00 | 36.74 |
| ATOM | 2611 | N | LYS | 523 | 70.827 | 25.849 | 12.193 | 1.00 | 38.60 |
| ATOM | 2612 | CA | LYS | 523 | 69.970 | 25.327 | 13.252 | 1.00 | 37.77 |
| ATOM | 2613 | CB | LYS | 523 | 68.628 | 26.053 | 13.273 | 1.00 | 44.52 |
| ATOM | 2614 | CG | LYS | 523 | 67.665 | 25.562 | 14.355 | 1.00 | 51.14 |
| ATOM | 2615 | CD | LYS | 523 | 66.380 | 24.983 | 13.756 | 1.00 | 57.39 |
| ATOM | 2616 | CE | LYS | 523 | 65.499 | 24.376 | 14.852 | 1.00 | 59.17 |
| ATOM | 2617 | NZ | LYS | 523 | 64.365 | 23.553 | 14.327 | 1.00 | 62.68 |
| ATOM | 2618 | C | LYS | 523 | 69.751 | 23.849 | 13.002 | 1.00 | 34.63 |
| ATOM | 2619 | O | LYS | 523 | 69.817 | 23.041 | 13.931 | 1.00 | 35.00 |
| ATOM | 2620 | N | ASP | 524 | 69.496 | 23.495 | 11.746 | 1.00 | 31.60 |
| ATOM | 2621 | CA | ASP | 524 | 69.293 | 22.100 | 11.367 | 1.00 | 29.05 |
| ATOM | 2622 | CB | ASP | 524 | 69.002 | 21.975 | 9.871 | 1.00 | 29.60 |
| ATOM | 2623 | CG | ASP | 524 | 67.695 | 22.626 | 9.472 | 1.00 | 31.90 |
| ATOM | 2624 | OD1 | ASP | 524 | 66.666 | 22.368 | 10.130 | 1.00 | 38.83 |
| ATOM | 2625 | OD2 | ASP | 524 | 67.687 | 23.383 | 8.485 | 1.00 | 29.79 |
| ATOM | 2626 | C | ASP | 524 | 70.558 | 21.317 | 11.696 | 1.00 | 28.02 |
| ATOM | 2627 | O | ASP | 524 | 70.494 | 20.201 | 12.212 | 1.00 | 28.12 |
| ATOM | 2628 | N | LEU | 525 | 71.709 | 21.899 | 11.378 | 1.00 | 28.32 |
| ATOM | 2629 | CA | LEU | 525 | 72.971 | 21.231 | 11.677 | 1.00 | 27.71 |
| ATOM | 2630 | CB | LEU | 525 | 74.173 | 22.085 | 11.257 | 1.00 | 22.53 |
| ATOM | 2631 | CG | LEU | 525 | 75.548 | 21.490 | 11.602 | 1.00 | 22.13 |
| ATOM | 2632 | CD1 | LEU | 525 | 75.677 | 20.082 | 11.019 | 1.00 | 19.92 |
| ATOM | 2633 | CD2 | LEU | 525 | 76.673 | 22.401 | 11.147 | 1.00 | 18.60 |
| ATOM | 2634 | C | LEU | 525 | 73.007 | 20.952 | 13.162 | 1.00 | 27.44 |
| ATOM | 2635 | O | LEU | 525 | 73.227 | 19.817 | 13.577 | 1.00 | 29.73 |
| ATOM | 2636 | N | SER | 526 | 72.689 | 21.976 | 13.947 | 1.00 | 29.09 |
| ATOM | 2637 | CA | SER | 526 | 72.672 | 21.891 | 15.412 | 1.00 | 30.83 |
| ATOM | 2638 | CB | SER | 526 | 72.222 | 23.230 | 16.006 | 1.00 | 34.25 |
| ATOM | 2639 | OG | SER | 526 | 71.966 | 23.147 | 17.397 | 1.00 | 40.67 |
| ATOM | 2640 | C | SER | 526 | 71.765 | 20.777 | 15.931 | 1.00 | 29.32 |
| ATOM | 2641 | O | SER | 526 | 72.055 | 20.133 | 16.954 | 1.00 | 28.94 |
| ATOM | 2642 | N | ASP | 527 | 70.644 | 20.587 | 15.242 | 1.00 | 26.54 |
| ATOM | 2643 | CA | ASP | 527 | 69.681 | 19.558 | 15.601 | 1.00 | 27.00 |
| ATOM | 2644 | CB | ASP | 527 | 68.392 | 19.798 | 14.829 | 1.00 | 25.91 |
| ATOM | 2645 | CG | ASP | 527 | 67.640 | 21.052 | 15.290 | 1.00 | 29.22 |
| ATOM | 2646 | OD1 | ASP | 527 | 68.016 | 21.662 | 16.320 | 1.00 | 26.80 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2647 | OD2 | ASP | 527 | 66.660 | 21.425 | 14.605 | 1.00 | 33.85 |
| ATOM | 2648 | C | ASP | 527 | 70.231 | 18.155 | 15.325 | 1.00 | 28.34 |
| ATOM | 2649 | O | ASP | 527 | 70.058 | 17.240 | 16.130 | 1.00 | 28.36 |
| ATOM | 2650 | N | LEU | 528 | 70.884 | 17.982 | 14.177 | 1.00 | 29.50 |
| ATOM | 2651 | CA | LEU | 528 | 71.448 | 16.680 | 13.830 | 1.00 | 30.48 |
| ATOM | 2652 | CB | LEU | 528 | 71.915 | 16.651 | 12.366 | 1.00 | 27.89 |
| ATOM | 2653 | CG | LEU | 528 | 72.443 | 15.305 | 11.832 | 1.00 | 26.48 |
| ATOM | 2654 | CD1 | LEU | 528 | 71.468 | 14.154 | 12.148 | 1.00 | 21.52 |
| ATOM | 2655 | CD2 | LEU | 528 | 72.722 | 15.383 | 10.333 | 1.00 | 20.23 |
| ATOM | 2656 | C | LEU | 528 | 72.583 | 16.308 | 14.804 | 1.00 | 31.69 |
| ATOM | 2657 | O | LEU | 528 | 72.688 | 15.145 | 15.222 | 1.00 | 30.09 |
| ATOM | 2658 | N | ILE | 529 | 73.397 | 17.298 | 15.195 | 1.00 | 30.79 |
| ATOM | 2659 | CA | ILE | 529 | 74.503 | 17.082 | 16.140 | 1.00 | 28.88 |
| ATOM | 2660 | CB | ILE | 529 | 75.398 | 18.310 | 16.278 | 1.00 | 25.69 |
| ATOM | 2661 | CG2 | ILE | 529 | 76.541 | 18.007 | 17.217 | 1.00 | 20.54 |
| ATOM | 2662 | CG1 | ILE | 529 | 75.960 | 18.727 | 14.941 | 1.00 | 23.71 |
| ATOM | 2663 | CD1 | ILE | 529 | 76.981 | 19.831 | 15.035 | 1.00 | 24.21 |
| ATOM | 2664 | C | ILE | 529 | 73.951 | 16.767 | 17.533 | 1.00 | 31.52 |
| ATOM | 2665 | O | ILE | 529 | 74.439 | 15.850 | 18.213 | 1.00 | 30.66 |
| ATOM | 2666 | N | SER | 530 | 72.917 | 17.500 | 17.947 | 1.00 | 29.79 |
| ATOM | 2667 | CA | SER | 530 | 72.315 | 17.257 | 19.244 | 1.00 | 32.03 |
| ATOM | 2668 | CB | SER | 530 | 71.176 | 18.239 | 19.492 | 1.00 | 38.91 |
| ATOM | 2669 | OG | SER | 530 | 70.266 | 18.231 | 18.412 | 1.00 | 49.86 |
| ATOM | 2670 | C | SER | 530 | 71.795 | 15.819 | 19.316 | 1.00 | 30.10 |
| ATOM | 2671 | O | SER | 530 | 71.921 | 15.154 | 20.353 | 1.00 | 31.31 |
| ATOM | 2672 | N | GLU | 531 | 71.185 | 15.350 | 18.231 | 1.00 | 27.18 |
| ATOM | 2673 | CA | GLU | 531 | 70.671 | 13.989 | 18.180 | 1.00 | 27.89 |
| ATOM | 2674 | CB | GLU | 531 | 69.923 | 13.744 | 16.881 | 1.00 | 31.29 |
| ATOM | 2675 | CG | GLU | 531 | 69.434 | 12.324 | 16.769 | 1.00 | 30.43 |
| ATOM | 2676 | CD | GLU | 531 | 68.717 | 12.040 | 15.486 | 1.00 | 30.67 |
| ATOM | 2677 | OE1 | GLU | 531 | 68.293 | 10.892 | 15.317 | 1.00 | 37.79 |
| ATOM | 2678 | OE2 | GLU | 531 | 68.571 | 12.941 | 14.643 | 1.00 | 34.20 |
| ATOM | 2679 | C | GLU | 531 | 71.765 | 12.929 | 18.348 | 1.00 | 26.67 |
| ATOM | 2680 | O | GLU | 531 | 71.604 | 11.986 | 19.119 | 1.00 | 24.33 |
| ATOM | 2681 | N | MET | 532 | 72.851 | 13.074 | 17.595 | 1.00 | 28.93 |
| ATOM | 2682 | CA | MET | 532 | 74.000 | 12.156 | 17.644 | 1.00 | 28.35 |
| ATOM | 2683 | CB | MET | 532 | 75.073 | 12.637 | 16.659 | 1.00 | 29.48 |
| ATOM | 2684 | CG | MET | 532 | 76.458 | 12.034 | 16.827 | 1.00 | 25.84 |
| ATOM | 2685 | SD | MET | 532 | 77.650 | 12.692 | 15.582 | 1.00 | 30.60 |
| ATOM | 2686 | CE | MET | 532 | 77.831 | 14.373 | 16.151 | 1.00 | 20.10 |
| ATOM | 2687 | C | MET | 532 | 74.571 | 12.120 | 19.057 | 1.00 | 29.06 |
| ATOM | 2688 | O | MET | 532 | 74.876 | 11.053 | 19.589 | 1.00 | 28.22 |
| ATOM | 2689 | N | GLU | 533 | 74.640 | 13.289 | 19.688 | 1.00 | 28.61 |
| ATOM | 2690 | CA | GLU | 533 | 75.150 | 13.388 | 21.041 | 1.00 | 28.40 |
| ATOM | 2691 | CB | GLU | 533 | 75.340 | 14.846 | 21.429 | 1.00 | 29.34 |
| ATOM | 2692 | CG | GLU | 533 | 76.449 | 15.534 | 20.640 | 1.00 | 31.87 |
| ATOM | 2693 | CD | GLU | 533 | 77.822 | 14.923 | 20.892 | 1.00 | 35.10 |
| ATOM | 2694 | OE1 | GLU | 533 | 78.242 | 14.831 | 22.067 | 1.00 | 37.36 |
| ATOM | 2695 | OE2 | GLU | 533 | 78.490 | 14.543 | 19.913 | 1.00 | 37.71 |
| ATOM | 2696 | C | GLU | 533 | 74.211 | 12.684 | 22.023 | 1.00 | 31.03 |
| ATOM | 2697 | O | GLU | 533 | 74.651 | 11.936 | 22.906 | 1.00 | 30.76 |
| ATOM | 2698 | N | MET | 534 | 72.909 | 12.902 | 21.860 | 1.00 | 31.71 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2699 | CA | MET | 534 | 71.940 | 12.256 | 22.727 | 1.00 | 30.58 |
| ATOM | 2700 | CB | MET | 534 | 70.510 | 12.620 | 22.315 | 1.00 | 33.53 |
| ATOM | 2701 | CG | MET | 534 | 69.538 | 12.624 | 23.509 | 0.50 | 32.45 |
| ATOM | 2702 | SD | MET | 534 | 67.778 | 12.682 | 23.150 | 0.50 | 30.95 |
| ATOM | 2703 | CE | MET | 534 | 67.523 | 14.422 | 22.895 | 0.50 | 30.50 |
| ATOM | 2704 | C | MET | 534 | 72.158 | 10.752 | 22.616 | 1.00 | 28.44 |
| ATOM | 2705 | O | MET | 534 | 72.304 | 10.077 | 23.614 | 1.00 | 27.63 |
| ATOM | 2706 | N | MET | 535 | 72.216 | 10.232 | 21.395 | 1.00 | 30.00 |
| ATOM | 2707 | CA | MET | 535 | 72.448 | 8.800 | 21.176 | 1.00 | 29.38 |
| ATOM | 2708 | CB | MET | 535 | 72.626 | 8.483 | 19.690 | 1.00 | 25.41 |
| ATOM | 2709 | CG | MET | 535 | 71.395 | 8.753 | 18.893 | 1.00 | 25.06 |
| ATOM | 2710 | SD | MET | 535 | 71.468 | 7.917 | 17.344 | 1.00 | 27.17 |
| ATOM | 2711 | CE | MET | 535 | 71.439 | 9.227 | 16.247 | 1.00 | 33.70 |
| ATOM | 2712 | C | MET | 535 | 73.675 | 8.345 | 21.938 | 1.00 | 30.77 |
| ATOM | 2713 | O | MET | 535 | 73.681 | 7.254 | 22.534 | 1.00 | 27.49 |
| ATOM | 2714 | N | LYS | 536 | 74.710 | 9.183 | 21.916 | 1.00 | 32.72 |
| ATOM | 2715 | CA | LYS | 536 | 75.937 | 8.889 | 22.649 | 1.00 | 34.05 |
| ATOM | 2716 | CB | LYS | 536 | 76.995 | 9.964 | 22.401 | 1.00 | 32.69 |
| ATOM | 2717 | CG | LYS | 536 | 77.719 | 9.838 | 21.073 | 1.00 | 28.00 |
| ATOM | 2718 | CD | LYS | 536 | 78.732 | 10.956 | 20.941 | 1.00 | 29.61 |
| ATOM | 2719 | CE | LYS | 536 | 79.242 | 11.124 | 19.514 | 1.00 | 26.58 |
| ATOM | 2720 | NZ | LYS | 536 | 80.020 | 12.389 | 19.460 | 1.00 | 22.22 |
| ATOM | 2721 | C | LYS | 536 | 75.652 | 8.769 | 24.145 | 1.00 | 34.80 |
| ATOM | 2722 | O | LYS | 536 | 76.004 | 7.763 | 24.750 | 1.00 | 34.44 |
| ATOM | 2723 | N | MET | 537 | 74.958 | 9.749 | 24.716 | 1.00 | 34.66 |
| ATOM | 2724 | CA | MET | 537 | 74.634 | 9.724 | 26.131 | 1.00 | 37.25 |
| ATOM | 2725 | CB | MET | 537 | 73.951 | 11.034 | 26.549 | 1.00 | 46.08 |
| ATOM | 2726 | CG | MET | 537 | 74.862 | 12.272 | 26.619 | 1.00 | 57.95 |
| ATOM | 2727 | SD | MET | 537 | 76.159 | 12.203 | 27.919 | 1.00 | 66.50 |
| ATOM | 2728 | CE | MET | 537 | 75.287 | 12.873 | 29.377 | 1.00 | 64.52 |
| ATOM | 2729 | C | MET | 537 | 73.749 | 8.537 | 26.523 | 1.00 | 36.05 |
| ATOM | 2730 | O | MET | 537 | 74.021 | 7.865 | 27.514 | 1.00 | 36.71 |
| ATOM | 2731 | N | ILE | 538 | 72.730 | 8.255 | 25.719 | 1.00 | 33.77 |
| ATOM | 2732 | CA | ILE | 538 | 71.804 | 7.160 | 26.007 | 1.00 | 30.52 |
| ATOM | 2733 | CB | ILE | 538 | 70.616 | 7.172 | 25.012 | 1.00 | 28.15 |
| ATOM | 2734 | CG2 | ILE | 538 | 69.780 | 5.899 | 25.122 | 1.00 | 26.08 |
| ATOM | 2735 | CG1 | ILE | 538 | 69.729 | 8.377 | 25.289 | 1.00 | 26.24 |
| ATOM | 2736 | CD1 | ILE | 538 | 68.644 | 8.558 | 24.256 | 1.00 | 26.87 |
| ATOM | 2737 | C | ILE | 538 | 72.399 | 5.750 | 26.100 | 1.00 | 30.05 |
| ATOM | 2738 | O | ILE | 538 | 71.984 | 4.950 | 26.941 | 1.00 | 31.57 |
| ATOM | 2739 | N | GLY | 539 | 73.320 | 5.424 | 25.211 | 1.00 | 30.34 |
| ATOM | 2740 | CA | GLY | 539 | 73.910 | 4.103 | 25.249 | 1.00 | 28.22 |
| ATOM | 2741 | C | GLY | 539 | 73.158 | 3.094 | 24.408 | 1.00 | 31.25 |
| ATOM | 2742 | O | GLY | 539 | 72.050 | 3.359 | 23.935 | 1.00 | 32.88 |
| ATOM | 2743 | N | LYS | 540 | 73.781 | 1.933 | 24.221 | 1.00 | 31.96 |
| ATOM | 2744 | CA | LYS | 540 | 73.222 | 0.845 | 23.416 | 1.00 | 33.40 |
| ATOM | 2745 | CB | LYS | 540 | 74.342 | -0.023 | 22.878 | 1.00 | 31.53 |
| ATOM | 2746 | CG | LYS | 540 | 75.177 | 0.645 | 21.846 | 1.00 | 37.05 |
| ATOM | 2747 | CD | LYS | 540 | 76.273 | -0.266 | 21.361 | 1.00 | 40.15 |
| ATOM | 2748 | CE | LYS | 540 | 77.143 | 0.480 | 20.363 | 1.00 | 46.84 |
| ATOM | 2749 | NZ | LYS | 540 | 76.374 | 0.920 | 19.152 | 1.00 | 48.60 |
| ATOM | 2750 | C | LYS | 540 | 72.183 | -0.090 | 24.023 | 1.00 | 36.22 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2751 | O | LYS | 540 | 72.237 | -0.430 | 25.215 | 1.00 | 40.10 |
| ATOM | 2752 | N | HIS | 541 | 71.254 | -0.521 | 23.175 | 1.00 | 34.86 |
| ATOM | 2753 | CA | HIS | 541 | 70.223 | -1.486 | 23.535 | 1.00 | 33.96 |
| ATOM | 2754 | CB | HIS | 541 | 69.064 | -0.860 | 24.293 | 1.00 | 31.57 |
| ATOM | 2755 | CG | HIS | 541 | 68.127 | -1.862 | 24.890 | 1.00 | 32.28 |
| ATOM | 2756 | CD2 | HIS | 541 | 68.127 | -2.482 | 26.093 | 1.00 | 32.39 |
| ATOM | 2757 | ND1 | HIS | 541 | 67.086 | -2.411 | 24.177 | 1.00 | 30.10 |
| ATOM | 2758 | CE1 | HIS | 541 | 66.489 | -3.329 | 24.911 | 1.00 | 33.35 |
| ATOM | 2759 | NE2 | HIS | 541 | 67.096 | -3.384 | 26.081 | 1.00 | 30.46 |
| ATOM | 2760 | C | HIS | 541 | 69.720 | -2.206 | 22.275 | 1.00 | 35.33 |
| ATOM | 2761 | O | HIS | 541 | 69.648 | -1.614 | 21.200 | 1.00 | 34.87 |
| ATOM | 2762 | N | LYS | 542 | 69.348 | -3.478 | 22.430 | 1.00 | 35.42 |
| ATOM | 2763 | CA | LYS | 542 | 68.908 | -4.311 | 21.306 | 1.00 | 32.02 |
| ATOM | 2764 | CB | LYS | 542 | 68.715 | -5.766 | 21.753 | 1.00 | 30.96 |
| ATOM | 2765 | C | LYS | 542 | 67.652 | -3.848 | 20.614 | 1.00 | 30.02 |
| ATOM | 2766 | O | LYS | 542 | 67.474 | -4.058 | 19.417 | 1.00 | 29.10 |
| ATOM | 2767 | N | ASN | 543 | 66.778 | -3.212 | 21.369 | 1.00 | 28.54 |
| ATOM | 2768 | CA | ASN | 543 | 65.529 | -2.754 | 20.803 | 1.00 | 28.20 |
| ATOM | 2769 | CB | ASN | 543 | 64.372 | -3.241 | 21.660 | 1.00 | 29.73 |
| ATOM | 2770 | CG | ASN | 543 | 64.387 | -4.739 | 21.840 | 1.00 | 30.74 |
| ATOM | 2771 | OD1 | ASN | 543 | 64.732 | -5.242 | 22.909 | 1.00 | 32.96 |
| ATOM | 2772 | ND2 | ASN | 543 | 64.053 | -5.462 | 20.787 | 1.00 | 29.58 |
| ATOM | 2773 | C | ASN | 543 | 65.426 | -1.257 | 20.529 | 1.00 | 28.06 |
| ATOM | 2774 | O | ASN | 543 | 64.342 | -0.679 | 20.647 | 1.00 | 28.86 |
| ATOM | 2775 | N | ILE | 544 | 66.546 | -0.635 | 20.168 | 1.00 | 26.70 |
| ATOM | 2776 | CA | ILE | 544 | 66.582 | 0.794 | 19.833 | 1.00 | 26.81 |
| ATOM | 2777 | CB | ILE | 544 | 67.052 | 1.721 | 21.019 | 1.00 | 24.75 |
| ATOM | 2778 | CG2 | ILE | 544 | 66.338 | 1.353 | 22.306 | 1.00 | 20.02 |
| ATOM | 2779 | CG1 | ILE | 544 | 68.568 | 1.614 | 21.234 | 1.00 | 23.73 |
| ATOM | 2780 | CD1 | ILE | 544 | 69.105 | 2.531 | 22.332 | 1.00 | 21.64 |
| ATOM | 2781 | C | ILE | 544 | 67.582 | 0.901 | 18.680 | 1.00 | 27.95 |
| ATOM | 2782 | O | ILE | 544 | 68.388 | -0.008 | 18.480 | 1.00 | 26.80 |
| ATOM | 2783 | N | ILE | 545 | 67.449 | 1.940 | 17.849 | 1.00 | 29.22 |
| ATOM | 2784 | CA | ILE | 545 | 68.376 | 2.163 | 16.745 | 1.00 | 27.14 |
| ATOM | 2785 | CB | ILE | 545 | 67.824 | 3.164 | 15.709 | 1.00 | 26.10 |
| ATOM | 2786 | CG2 | ILE | 545 | 68.920 | 3.556 | 14.731 | 1.00 | 24.70 |
| ATOM | 2787 | CG1 | ILE | 545 | 66.625 | 2.568 | 14.955 | 1.00 | 23.78 |
| ATOM | 2788 | CD1 | ILE | 545 | 66.988 | 1.326 | 14.117 | 1.00 | 22.15 |
| ATOM | 2789 | C | ILE | 545 | 69.631 | 2.718 | 17.401 | 1.00 | 28.14 |
| ATOM | 2790 | O | ILE | 545 | 69.586 | 3.752 | 18.068 | 1.00 | 28.21 |
| ATOM | 2791 | N | ASN | 546 | 70.740 | 2.011 | 17.221 | 1.00 | 28.40 |
| ATOM | 2792 | CA | ASN | 546 | 72.004 | 2.382 | 17.822 | 1.00 | 28.49 |
| ATOM | 2793 | CB | ASN | 546 | 72.709 | 1.122 | 18.345 | 1.00 | 27.05 |
| ATOM | 2794 | CG | ASN | 546 | 71.956 | 0.463 | 19.470 | 1.00 | 27.29 |
| ATOM | 2795 | OD1 | ASN | 546 | 71.793 | 1.031 | 20.540 | 1.00 | 29.92 |
| ATOM | 2796 | ND2 | ASN | 546 | 71.472 | -0.740 | 19.235 | 1.00 | 24.63 |
| ATOM | 2797 | C | ASN | 546 | 72.982 | 3.124 | 16.941 | 1.00 | 28.39 |
| ATOM | 2798 | O | ASN | 546 | 73.045 | 2.894 | 15.732 | 1.00 | 29.62 |
| ATOM | 2799 | N | LEU | 547 | 73.774 | 3.982 | 17.579 | 1.00 | 29.91 |
| ATOM | 2800 | CA | LEU | 547 | 74.828 | 4.750 | 16.925 | 1.00 | 30.68 |
| ATOM | 2801 | CB | LEU | 547 | 75.297 | 5.898 | 17.837 | 1.00 | 25.28 |
| ATOM | 2802 | CG | LEU | 547 | 76.367 | 6.828 | 17.267 | 1.00 | 24.81 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2803 | CD1 | LEU | 547 | 75.868 | 7.524 | 15.990 | 1.00 | 22.25 |
| ATOM | 2804 | CD2 | LEU | 547 | 76.716 | 7.853 | 18.313 | 1.00 | 24.17 |
| ATOM | 2805 | C | LEU | 547 | 76.016 | 3.812 | 16.629 | 1.00 | 31.67 |
| ATOM | 2806 | O | LEU | 547 | 76.481 | 3.090 | 17.509 | 1.00 | 31.34 |
| ATOM | 2807 | N | LEU | 548 | 76.475 | 3.823 | 15.380 | 1.00 | 30.60 |
| ATOM | 2808 | CA | LEU | 548 | 77.594 | 2.995 | 14.955 | 1.00 | 29.31 |
| ATOM | 2809 | CB | LEU | 548 | 77.197 | 2.165 | 13.729 | 1.00 | 25.94 |
| ATOM | 2810 | CG | LEU | 548 | 75.968 | 1.247 | 13.883 | 1.00 | 28.78 |
| ATOM | 2811 | CD1 | LEU | 548 | 75.848 | 0.360 | 12.659 | 1.00 | 27.14 |
| ATOM | 2812 | CD2 | LEU | 548 | 76.049 | 0.392 | 15.149 | 1.00 | 23.72 |
| ATOM | 2813 | C | LEU | 548 | 78.850 | 3.821 | 14.644 | 1.00 | 31.60 |
| ATOM | 2814 | O | LEU | 548 | 79.967 | 3.330 | 14.753 | 1.00 | 32.65 |
| ATOM | 2815 | N | GLY | 549 | 78.665 | 5.076 | 14.248 | 1.00 | 32.22 |
| ATOM | 2816 | CA | GLY | 549 | 79.795 | 5.928 | 13.937 | 1.00 | 31.40 |
| ATOM | 2817 | C | GLY | 549 | 79.344 | 7.267 | 13.391 | 1.00 | 30.78 |
| ATOM | 2818 | O | GLY | 549 | 78.140 | 7.536 | 13.291 | 1.00 | 29.84 |
| ATOM | 2819 | N | ALA | 550 | 80.320 | 8.099 | 13.045 | 1.00 | 31.88 |
| ATOM | 2820 | CA | ALA | 550 | 80.073 | 9.416 | 12.485 | 1.00 | 30.14 |
| ATOM | 2821 | CB | ALA | 550 | 79.634 | 10.382 | 13.590 | 1.00 | 31.08 |
| ATOM | 2822 | C | ALA | 550 | 81.291 | 9.978 | 11.742 | 1.00 | 28.78 |
| ATOM | 2823 | O | ALA | 550 | 82.447 | 9.705 | 12.102 | 1.00 | 26.39 |
| ATOM | 2824 | N | CYS | 551 | 81.011 | 10.690 | 10.651 | 1.00 | 28.48 |
| ATOM | 2825 | CA | CYS | 551 | 82.012 | 11.391 | 9.846 | 1.00 | 23.69 |
| ATOM | 2826 | CB | CYS | 551 | 81.825 | 11.128 | 8.352 | 1.00 | 24.18 |
| ATOM | 2827 | SG | CYS | 551 | 81.870 | 9.395 | 7.840 | 1.00 | 28.40 |
| ATOM | 2828 | C | CYS | 551 | 81.612 | 12.847 | 10.127 | 1.00 | 20.99 |
| ATOM | 2829 | O | CYS | 551 | 80.561 | 13.282 | 9.684 | 1.00 | 22.11 |
| ATOM | 2830 | N | THR | 552 | 82.357 | 13.524 | 10.996 | 1.00 | 20.18 |
| ATOM | 2831 | CA | THR | 552 | 82.073 | 14.914 | 11.349 | 1.00 | 22.79 |
| ATOM | 2832 | CB | THR | 552 | 82.090 | 15.080 | 12.874 | 1.00 | 23.16 |
| ATOM | 2833 | OG1 | THR | 552 | 83.408 | 14.803 | 13.363 | 1.00 | 23.52 |
| ATOM | 2834 | CG2 | THR | 552 | 81.125 | 14.112 | 13.529 | 1.00 | 25.31 |
| ATOM | 2835 | C | THR | 552 | 83.138 | 15.886 | 10.824 | 1.00 | 24.74 |
| ATOM | 2836 | O | THR | 552 | 82.939 | 17.103 | 10.782 | 1.00 | 22.75 |
| ATOM | 2837 | N | GLN | 553 | 84.276 | 15.334 | 10.431 | 1.00 | 26.82 |
| ATOM | 2838 | CA | GLN | 553 | 85.387 | 16.153 | 9.980 | 1.00 | 26.99 |
| ATOM | 2839 | CB | GLN | 553 | 86.686 | 15.627 | 10.602 | 1.00 | 26.40 |
| ATOM | 2840 | CG | GLN | 553 | 86.632 | 15.494 | 12.141 | 1.00 | 22.69 |
| ATOM | 2841 | CD | GLN | 553 | 86.438 | 16.836 | 12.823 | 1.00 | 25.90 |
| ATOM | 2842 | OE1 | GLN | 553 | 87.259 | 17.729 | 12.656 | 1.00 | 29.03 |
| ATOM | 2843 | NE2 | GLN | 553 | 85.351 | 16.994 | 13.566 | 1.00 | 23.53 |
| ATOM | 2844 | C | GLN | 553 | 85.502 | 16.216 | 8.466 | 1.00 | 26.23 |
| ATOM | 2845 | O | GLN | 553 | 85.177 | 15.259 | 7.779 | 1.00 | 30.00 |
| ATOM | 2846 | N | ASP | 554 | 85.863 | 17.394 | 7.968 | 1.00 | 26.54 |
| ATOM | 2847 | CA | ASP | 554 | 86.084 | 17.631 | 6.531 | 1.00 | 28.38 |
| ATOM | 2848 | CB | ASP | 554 | 87.410 | 17.031 | 6.105 | 1.00 | 26.78 |
| ATOM | 2849 | CG | ASP | 554 | 88.538 | 17.570 | 6.912 | 1.00 | 31.53 |
| ATOM | 2850 | OD1 | ASP | 554 | 88.789 | 18.795 | 6.823 | 1.00 | 35.18 |
| ATOM | 2851 | OD2 | ASP | 554 | 89.141 | 16.795 | 7.665 | 1.00 | 29.04 |
| ATOM | 2852 | C | ASP | 554 | 85.011 | 17.221 | 5.545 | 1.00 | 29.14 |
| ATOM | 2853 | O | ASP | 554 | 85.278 | 16.468 | 4.610 | 1.00 | 31.22 |
| ATOM | 2854 | N | GLY | 555 | 83.824 | 17.793 | 5.709 | 1.00 | 31.20 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2855 | CA | GLY | 555 | 82.723 | 17.490 | 4.811 | 1.00 | 28.83 |
| ATOM | 2856 | C | GLY | 555 | 81.446 | 17.413 | 5.602 | 1.00 | 24.84 |
| ATOM | 2857 | O | GLY | 555 | 81.448 | 17.647 | 6.814 | 1.00 | 21.78 |
| ATOM | 2858 | N | PRO | 556 | 80.317 | 17.093 | 4.953 | 1.00 | 24.29 |
| ATOM | 2859 | CD | PRO | 556 | 80.213 | 16.781 | 3.510 | 1.00 | 19.37 |
| ATOM | 2860 | CA | PRO | 556 | 79.010 | 16.973 | 5.615 | 1.00 | 25.11 |
| ATOM | 2861 | CB | PRO | 556 | 78.107 | 16.497 | 4.477 | 1.00 | 22.88 |
| ATOM | 2862 | CG | PRO | 556 | 79.077 | 15.832 | 3.485 | 1.00 | 23.50 |
| ATOM | 2863 | C | PRO | 556 | 79.006 | 15.982 | 6.777 | 1.00 | 27.67 |
| ATOM | 2864 | O | PRO | 556 | 79.676 | 14.947 | 6.736 | 1.00 | 27.13 |
| ATOM | 2865 | N | LEU | 557 | 78.253 | 16.297 | 7.820 | 1.00 | 29.27 |
| ATOM | 2866 | CA | LEU | 557 | 78.164 | 15.405 | 8.972 | 1.00 | 31.19 |
| ATOM | 2867 | CB | LEU | 557 | 77.583 | 16.130 | 10.188 | 1.00 | 29.94 |
| ATOM | 2868 | CG | LEU | 557 | 77.019 | 15.260 | 11.323 | 1.00 | 26.87 |
| ATOM | 2869 | CD1 | LEU | 557 | 78.131 | 14.540 | 12.062 | 1.00 | 23.83 |
| ATOM | 2870 | CD2 | LEU | 557 | 76.237 | 16.146 | 12.275 | 1.00 | 23.80 |
| ATOM | 2871 | C | LEU | 557 | 77.291 | 14.193 | 8.651 | 1.00 | 31.97 |
| ATOM | 2872 | O | LEU | 557 | 76.158 | 14.332 | 8.184 | 1.00 | 31.18 |
| ATOM | 2873 | N | TYR | 558 | 77.857 | 13.010 | 8.882 | 1.00 | 31.12 |
| ATOM | 2874 | CA | TYR | 558 | 77.145 | 11.767 | 8.664 | 1.00 | 28.86 |
| ATOM | 2875 | CB | TYR | 558 | 77.905 | 10.869 | 7.694 | 1.00 | 28.58 |
| ATOM | 2876 | CG | TYR | 558 | 78.017 | 11.395 | 6.281 | 1.00 | 32.33 |
| ATOM | 2877 | CD1 | TYR | 558 | 79.034 | 10.962 | 5.443 | 1.00 | 35.23 |
| ATOM | 2878 | CE1 | TYR | 558 | 79.161 | 11.447 | 4.151 | 1.00 | 37.54 |
| ATOM | 2879 | CD2 | TYR | 558 | 77.123 | 12.336 | 5.787 | 1.00 | 35.27 |
| ATOM | 2880 | CE2 | TYR | 558 | 77.248 | 12.832 | 4.493 | 1.00 | 36.43 |
| ATOM | 2881 | CZ | TYR | 558 | 78.276 | 12.382 | 3.680 | 1.00 | 37.05 |
| ATOM | 2882 | OH | TYR | 558 | 78.423 | 12.869 | 2.394 | 1.00 | 39.97 |
| ATOM | 2883 | C | TYR | 558 | 77.000 | 11.071 | 10.004 | 1.00 | 26.63 |
| ATOM | 2884 | O | TYR | 558 | 77.985 | 10.885 | 10.725 | 1.00 | 24.67 |
| ATOM | 2885 | N | VAL | 559 | 75.756 | 10.774 | 10.365 | 1.00 | 28.15 |
| ATOM | 2886 | CA | VAL | 559 | 75.429 | 10.070 | 11.610 | 1.00 | 27.70 |
| ATOM | 2887 | CB | VAL | 559 | 74.262 | 10.770 | 12.372 | 1.00 | 26.63 |
| ATOM | 2888 | CG1 | VAL | 559 | 73.876 | 9.959 | 13.603 | 1.00 | 24.70 |
| ATOM | 2889 | CG2 | VAL | 559 | 74.673 | 12.186 | 12.792 | 1.00 | 26.71 |
| ATOM | 2890 | C | VAL | 559 | 75.061 | 8.635 | 11.205 | 1.00 | 27.08 |
| ATOM | 2891 | O | VAL | 559 | 73.965 | 8.357 | 10.710 | 1.00 | 25.39 |
| ATOM | 2892 | N | ILE | 560 | 76.002 | 7.729 | 11.399 | 1.00 | 28.25 |
| ATOM | 2893 | CA | ILE | 560 | 75.820 | 6.335 | 11.000 | 1.00 | 29.62 |
| ATOM | 2894 | CB | ILE | 560 | 77.225 | 5.682 | 10.678 | 1.00 | 30.06 |
| ATOM | 2895 | CG2 | ILE | 560 | 77.045 | 4.279 | 10.101 | 1.00 | 31.58 |
| ATOM | 2896 | CG1 | ILE | 560 | 78.004 | 6.557 | 9.686 | 1.00 | 27.50 |
| ATOM | 2897 | CD1 | ILE | 560 | 79.492 | 6.239 | 9.629 | 1.00 | 23.31 |
| ATOM | 2898 | C | ILE | 560 | 75.075 | 5.488 | 12.032 | 1.00 | 29.88 |
| ATOM | 2899 | O | ILE | 560 | 75.586 | 5.234 | 13.130 | 1.00 | 27.32 |
| ATOM | 2900 | N | VAL | 561 | 73.857 | 5.078 | 11.687 | 1.00 | 29.09 |
| ATOM | 2901 | CA | VAL | 561 | 73.053 | 4.228 | 12.568 | 1.00 | 28.70 |
| ATOM | 2902 | CB | VAL | 561 | 71.743 | 4.932 | 13.037 | 1.00 | 25.29 |
| ATOM | 2903 | CG1 | VAL | 561 | 72.072 | 6.139 | 13.872 | 1.00 | 22.91 |
| ATOM | 2904 | CG2 | VAL | 561 | 70.887 | 5.312 | 11.870 | 1.00 | 22.38 |
| ATOM | 2905 | C | VAL | 561 | 72.731 | 2.848 | 11.945 | 1.00 | 27.99 |
| ATOM | 2906 | O | VAL | 561 | 73.052 | 2.590 | 10.783 | 1.00 | 27.88 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2907 | N | GLU | 562 | 72.143 | 1.969 | 12.754 | 1.00 | 27.38 |
| ATOM | 2908 | CA | GLU | 562 | 71.759 | 0.616 | 12.347 | 1.00 | 28.01 |
| ATOM | 2909 | CB | GLU | 562 | 71.246 | -0.161 | 13.555 | 1.00 | 25.37 |
| ATOM | 2910 | CG | GLU | 562 | 72.322 | -0.487 | 14.570 | 1.00 | 29.22 |
| ATOM | 2911 | CD | GLU | 562 | 71.785 | -1.190 | 15.796 | 1.00 | 30.94 |
| ATOM | 2912 | OE1 | GLU | 562 | 72.440 | -2.135 | 16.271 | 1.00 | 34.82 |
| ATOM | 2913 | OE2 | GLU | 562 | 70.716 | -0.795 | 16.297 | 1.00 | 32.77 |
| ATOM | 2914 | C | GLU | 562 | 70.695 | 0.610 | 11.266 | 1.00 | 29.83 |
| ATOM | 2915 | O | GLU | 562 | 69.822 | 1.452 | 11.274 | 1.00 | 34.69 |
| ATOM | 2916 | N | TYR | 563 | 70.755 | -0.364 | 10.362 | 1.00 | 31.35 |
| ATOM | 2917 | CA | TYR | 563 | 69.806 | -0.527 | 9.255 | 1.00 | 33.79 |
| ATOM | 2918 | CB | TYR | 563 | 70.586 | -0.987 | 8.022 | 1.00 | 32.37 |
| ATOM | 2919 | CG | TYR | 563 | 69.759 | -1.232 | 6.778 | 1.00 | 31.70 |
| ATOM | 2920 | CD1 | TYR | 563 | 68.858 | -0.277 | 6.319 | 1.00 | 35.00 |
| ATOM | 2921 | CE1 | TYR | 563 | 68.101 | -0.490 | 5.161 | 1.00 | 35.62 |
| ATOM | 2922 | CD2 | TYR | 563 | 69.888 | -2.416 | 6.053 | 1.00 | 31.64 |
| ATOM | 2923 | CE2 | TYR | 563 | 69.138 | -2.644 | 4.894 | 1.00 | 32.96 |
| ATOM | 2924 | CZ | TYR | 563 | 68.242 | -1.674 | 4.462 | 1.00 | 36.20 |
| ATOM | 2925 | OH | TYR | 563 | 67.494 | -1.906 | 3.340 | 1.00 | 39.54 |
| ATOM | 2926 | C | TYR | 563 | 68.668 | -1.527 | 9.593 | 1.00 | 37.26 |
| ATOM | 2927 | O | TYR | 563 | 68.915 | -2.566 | 10.212 | 1.00 | 38.86 |
| ATOM | 2928 | N | ALA | 564 | 67.428 | -1.180 | 9.220 | 1.00 | 39.09 |
| ATOM | 2929 | CA | ALA | 564 | 66.256 | -2.027 | 9.467 | 1.00 | 37.64 |
| ATOM | 2930 | CB | ALA | 564 | 65.290 | -1.317 | 10.366 | 1.00 | 41.34 |
| ATOM | 2931 | C | ALA | 564 | 65.600 | -2.337 | 8.124 | 1.00 | 39.33 |
| ATOM | 2932 | O | ALA | 564 | 64.700 | -1.628 | 7.661 | 1.00 | 41.28 |
| ATOM | 2933 | N | SER | 565 | 66.033 | -3.432 | 7.515 | 1.00 | 40.21 |
| ATOM | 2934 | CA | SER | 565 | 65.567 | -3.867 | 6.202 | 1.00 | 40.22 |
| ATOM | 2935 | CB | SER | 565 | 66.302 | -5.133 | 5.808 | 1.00 | 38.50 |
| ATOM | 2936 | OG | SER | 565 | 66.174 | -6.084 | 6.847 | 1.00 | 37.66 |
| ATOM | 2937 | C | SER | 565 | 64.095 | -4.087 | 5.987 | 1.00 | 42.30 |
| ATOM | 2938 | O | SER | 565 | 63.657 | -4.155 | 4.840 | 1.00 | 46.83 |
| ATOM | 2939 | N | LYS | 566 | 63.322 | -4.248 | 7.054 | 1.00 | 42.84 |
| ATOM | 2940 | CA | LYS | 566 | 61.893 | -4.462 | 6.883 | 1.00 | 41.84 |
| ATOM | 2941 | CB | LYS | 566 | 61.455 | -5.681 | 7.684 | 1.00 | 44.88 |
| ATOM | 2942 | CG | LYS | 566 | 62.003 | -6.977 | 7.088 | 1.00 | 48.86 |
| ATOM | 2943 | CD | LYS | 566 | 61.929 | -8.148 | 8.040 | 1.00 | 51.41 |
| ATOM | 2944 | CE | LYS | 566 | 62.582 | -9.362 | 7.426 | 1.00 | 53.89 |
| ATOM | 2945 | NZ | LYS | 566 | 62.706 | -10.465 | 8.417 | 1.00 | 59.37 |
| ATOM | 2946 | C | LYS | 566 | 61.029 | -3.234 | 7.143 | 1.00 | 41.89 |
| ATOM | 2947 | O | LYS | 566 | 59.815 | -3.337 | 7.341 | 1.00 | 43.68 |
| ATOM | 2948 | N | GLY | 567 | 61.663 | -2.061 | 7.100 | 1.00 | 39.50 |
| ATOM | 2949 | CA | GLY | 567 | 60.956 | -0.808 | 7.291 | 1.00 | 36.69 |
| ATOM | 2950 | C | GLY | 567 | 60.306 | -0.640 | 8.644 | 1.00 | 35.86 |
| ATOM | 2951 | O | GLY | 567 | 60.727 | -1.265 | 9.614 | 1.00 | 35.90 |
| ATOM | 2952 | N | ASN | 568 | 59.296 | 0.218 | 8.711 | 1.00 | 35.45 |
| ATOM | 2953 | CA | ASN | 568 | 58.615 | 0.447 | 9.966 | 1.00 | 38.10 |
| ATOM | 2954 | CB | ASN | 568 | 57.961 | 1.839 | 10.029 | 1.00 | 40.77 |
| ATOM | 2955 | CG | ASN | 568 | 56.701 | 1.962 | 9.163 | 1.00 | 43.52 |
| ATOM | 2956 | OD1 | ASN | 568 | 55.718 | 1.241 | 9.338 | 1.00 | 44.01 |
| ATOM | 2957 | ND2 | ASN | 568 | 56.710 | 2.932 | 8.263 | 1.00 | 45.39 |
| ATOM | 2958 | C | ASN | 568 | 57.610 | -0.657 | 10.269 | 1.00 | 38.91 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2959 | O | ASN | 568 | 57.218 | -1.420 | 9.384 | 1.00 | 39.95 |
| ATOM | 2960 | N | LEU | 569 | 57.204 | -0.717 | 11.534 | 1.00 | 38.93 |
| ATOM | 2961 | CA | LEU | 569 | 56.256 | -1.692 | 12.047 | 1.00 | 36.49 |
| ATOM | 2962 | CB | LEU | 569 | 56.126 | -1.507 | 13.555 | 1.00 | 36.53 |
| ATOM | 2963 | CG | LEU | 569 | 55.150 | -2.417 | 14.290 | 1.00 | 35.27 |
| ATOM | 2964 | CD1 | LEU | 569 | 55.550 | -3.865 | 14.047 | 1.00 | 31.86 |
| ATOM | 2965 | CD2 | LEU | 569 | 55.148 | -2.067 | 15.768 | 1.00 | 35.00 |
| ATOM | 2966 | C | LEU | 569 | 54.875 | -1.622 | 11.391 | 1.00 | 37.19 |
| ATOM | 2967 | O | LEU | 569 | 54.231 | -2.654 | 11.175 | 1.00 | 38.40 |
| ATOM | 2968 | N | ARG | 570 | 54.386 | -0.420 | 11.101 | 1.00 | 36.63 |
| ATOM | 2969 | CA | ARG | 570 | 53.068 | -0.294 | 10.485 | 1.00 | 36.68 |
| ATOM | 2970 | CB | ARG | 570 | 52.739 | 1.168 | 10.188 | 1.00 | 37.76 |
| ATOM | 2971 | CG | ARG | 570 | 51.339 | 1.361 | 9.623 | 1.00 | 46.41 |
| ATOM | 2972 | CD | ARG | 570 | 51.210 | 2.680 | 8.889 | 1.00 | 56.33 |
| ATOM | 2973 | NE | ARG | 570 | 52.162 | 2.785 | 7.779 | 1.00 | 63.05 |
| ATOM | 2974 | CZ | ARG | 570 | 53.010 | 3.798 | 7.603 | 1.00 | 66.33 |
| ATOM | 2975 | NH1 | ARG | 570 | 53.032 | 4.809 | 8.468 | 1.00 | 65.15 |
| ATOM | 2976 | NH2 | ARG | 570 | 53.853 | 3.786 | 6.580 | 1.00 | 66.56 |
| ATOM | 2977 | C | ARG | 570 | 53.046 | -1.094 | 9.193 | 1.00 | 35.55 |
| ATOM | 2978 | O | ARG | 570 | 52.248 | -2.015 | 9.018 | 1.00 | 35.33 |
| ATOM | 2979 | N | GLU | 571 | 53.978 | -0.758 | 8.320 | 1.00 | 37.20 |
| ATOM | 2980 | CA | GLU | 571 | 54.128 | -1.401 | 7.030 | 1.00 | 38.32 |
| ATOM | 2981 | CB | GLU | 571 | 55.247 | -0.695 | 6.261 | 1.00 | 40.15 |
| ATOM | 2982 | CG | GLU | 571 | 55.001 | 0.803 | 6.152 | 1.00 | 49.09 |
| ATOM | 2983 | CD | GLU | 571 | 56.118 | 1.557 | 5.442 | 1.00 | 58.16 |
| ATOM | 2984 | OE1 | GLU | 571 | 57.279 | 1.073 | 5.421 | 1.00 | 61.41 |
| ATOM | 2985 | OE2 | GLU | 571 | 55.824 | 2.660 | 4.914 | 1.00 | 61.27 |
| ATOM | 2986 | C | GLU | 571 | 54.406 | -2.906 | 7.170 | 1.00 | 36.74 |
| ATOM | 2987 | O | GLU | 571 | 53.863 | -3.721 | 6.410 | 1.00 | 35.74 |
| ATOM | 2988 | N | TYR | 572 | 55.241 | -3.266 | 8.141 | 1.00 | 35.13 |
| ATOM | 2989 | CA | TYR | 572 | 55.591 | -4.665 | 8.401 | 1.00 | 37.12 |
| ATOM | 2990 | CB | TYR | 572 | 56.591 | -4.736 | 9.560 | 1.00 | 34.39 |
| ATOM | 2991 | CG | TYR | 572 | 56.984 | -6.128 | 10.029 | 1.00 | 33.48 |
| ATOM | 2992 | CD1 | TYR | 572 | 57.980 | -6.869 | 9.367 | 1.00 | 29.76 |
| ATOM | 2993 | CE1 | TYR | 572 | 58.394 | -8.119 | 9.845 | 1.00 | 27.14 |
| ATOM | 2994 | CD2 | TYR | 572 | 56.406 | -6.681 | 11.183 | 1.00 | 32.40 |
| ATOM | 2995 | CE2 | TYR | 572 | 56.814 | -7.931 | 11.669 | 1.00 | 30.83 |
| ATOM | 2996 | CZ | TYR | 572 | 57.807 | -8.641 | 10.995 | 1.00 | 33.73 |
| ATOM | 2997 | OH | TYR | 572 | 58.201 | -9.872 | 11.480 | 1.00 | 37.16 |
| ATOM | 2998 | C | TYR | 572 | 54.330 | -5.468 | 8.729 | 1.00 | 38.92 |
| ATOM | 2999 | O | TYR | 572 | 54.108 | -6.553 | 8.183 | 1.00 | 39.22 |
| ATOM | 3000 | N | LEU | 573 | 53.507 | -4.922 | 9.618 | 1.00 | 38.41 |
| ATOM | 3001 | CA | LEU | 573 | 52.261 | -5.563 | 10.016 | 1.00 | 37.56 |
| ATOM | 3002 | CB | LEU | 573 | 51.573 | -4.711 | 11.084 | 1.00 | 36.44 |
| ATOM | 3003 | CG | LEU | 573 | 52.270 | -4.617 | 12.437 | 1.00 | 33.91 |
| ATOM | 3004 | CD1 | LEU | 573 | 51.555 | -3.626 | 13.372 | 1.00 | 31.60 |
| ATOM | 3005 | CD2 | LEU | 573 | 52.313 | -6.024 | 13.003 | 1.00 | 30.78 |
| ATOM | 3006 | C | LEU | 573 | 51.315 | -5.738 | 8.826 | 1.00 | 37.51 |
| ATOM | 3007 | O | LEU | 573 | 50.847 | -6.836 | 8.539 | 1.00 | 36.70 |
| ATOM | 3008 | N | GLN | 574 | 51.045 | -4.643 | 8.125 | 1.00 | 40.10 |
| ATOM | 3009 | CA | GLN | 574 | 50.141 | -4.678 | 6.986 | 1.00 | 41.10 |
| ATOM | 3010 | CB | GLN | 574 | 49.938 | -3.272 | 6.439 | 1.00 | 40.12 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3011 | CG | GLN | 574 | 49.171 | -2.381 | 7.374 | 1.00 | 40.77 |
| ATOM | 3012 | CD | GLN | 574 | 49.079 | -0.987 | 6.852 | 1.00 | 43.90 |
| ATOM | 3013 | OE1 | GLN | 574 | 49.679 | -0.652 | 5.835 | 1.00 | 46.93 |
| ATOM | 3014 | NE2 | GLN | 574 | 48.357 | -0.143 | 7.558 | 1.00 | 46.85 |
| ATOM | 3015 | C | GLN | 574 | 50.546 | -5.638 | 5.875 | 1.00 | 41.31 |
| ATOM | 3016 | O | GLN | 574 | 49.699 | -6.323 | 5.309 | 1.00 | 44.33 |
| ATOM | 3017 | N | ALA | 575 | 51.840 | -5.735 | 5.601 | 1.00 | 41.46 |
| ATOM | 3018 | CA | ALA | 575 | 52.317 | -6.628 | 4.555 | 1.00 | 39.80 |
| ATOM | 3019 | CB | ALA | 575 | 53.745 | -6.301 | 4.218 | 1.00 | 40.58 |
| ATOM | 3020 | C | ALA | 575 | 52.197 | -8.096 | 4.947 | 1.00 | 40.86 |
| ATOM | 3021 | O | ALA | 575 | 52.527 | -8.975 | 4.165 | 1.00 | 41.50 |
| ATOM | 3022 | N | ARG | 576 | 51.757 | -8.359 | 6.168 | 1.00 | 42.47 |
| ATOM | 3023 | CA | ARG | 576 | 51.624 | -9.726 | 6.641 | 1.00 | 42.68 |
| ATOM | 3024 | CB | ARG | 576 | 52.679 | -9.988 | 7.716 | 1.00 | 41.04 |
| ATOM | 3025 | CG | ARG | 576 | 54.095 | -9.958 | 7.161 | 1.00 | 42.73 |
| ATOM | 3026 | CD | ARG | 576 | 55.156 | -9.943 | 8.257 | 1.00 | 45.59 |
| ATOM | 3027 | NE | ARG | 576 | 56.514 | -9.870 | 7.695 | 1.00 | 43.89 |
| ATOM | 3028 | CZ | ARG | 576 | 56.981 | -8.856 | 6.969 | 1.00 | 43.35 |
| ATOM | 3029 | NH1 | ARG | 576 | 56.219 | -7.803 | 6.703 | 1.00 | 44.85 |
| ATOM | 3030 | NH2 | ARG | 576 | 58.215 | -8.902 | 6.497 | 1.00 | 41.84 |
| ATOM | 3031 | C | ARG | 576 | 50.232 | -10.014 | 7.180 | 1.00 | 44.86 |
| ATOM | 3032 | O | ARG | 576 | 50.043 | -10.943 | 7.970 | 1.00 | 46.08 |
| ATOM | 3033 | N | ARG | 577 | 49.258 | -9.216 | 6.753 | 1.00 | 46.72 |
| ATOM | 3034 | CA | ARG | 577 | 47.877 | -9.401 | 7.196 | 1.00 | 47.61 |
| ATOM | 3035 | CB | ARG | 577 | 46.994 | -8.239 | 6.723 | 1.00 | 46.35 |
| ATOM | 3036 | CG | ARG | 577 | 47.101 | -6.995 | 7.581 | 1.00 | 47.71 |
| ATOM | 3037 | CD | ARG | 577 | 46.329 | -5.831 | 6.999 | 1.00 | 49.15 |
| ATOM | 3038 | NE | ARG | 577 | 46.213 | -4.735 | 7.957 | 1.00 | 53.23 |
| ATOM | 3039 | CZ | ARG | 577 | 45.584 | -3.587 | 7.725 | 1.00 | 54.38 |
| ATOM | 3040 | NH1 | ARG | 577 | 45.020 | -3.368 | 6.549 | 1.00 | 56.41 |
| ATOM | 3041 | NH2 | ARG | 577 | 45.481 | -2.676 | 8.686 | 1.00 | 58.13 |
| ATOM | 3042 | C | ARG | 577 | 47.298 | -10.740 | 6.743 | 1.00 | 47.36 |
| ATOM | 3043 | O | ARG | 577 | 47.246 | -11.031 | 5.550 | 1.00 | 48.52 |
| ATOM | 3044 | N | GLN | 594 | 53.349 | -13.948 | 7.960 | 1.00 | 68.05 |
| ATOM | 3045 | CA | GLN | 594 | 52.144 | -14.067 | 8.772 | 1.00 | 66.75 |
| ATOM | 3046 | CB | GLN | 594 | 51.259 | -15.220 | 8.277 | 1.00 | 66.87 |
| ATOM | 3047 | C | GLN | 594 | 52.535 | -14.284 | 10.233 | 1.00 | 64.71 |
| ATOM | 3048 | O | GLN | 594 | 53.192 | -15.264 | 10.580 | 1.00 | 64.86 |
| ATOM | 3049 | N | LEU | 595 | 52.159 | -13.335 | 11.074 | 1.00 | 61.14 |
| ATOM | 3050 | CA | LEU | 595 | 52.489 | -13.422 | 12.480 | 1.00 | 58.19 |
| ATOM | 3051 | CB | LEU | 595 | 52.599 | -12.008 | 13.056 | 1.00 | 56.33 |
| ATOM | 3052 | CG | LEU | 595 | 53.532 | -11.147 | 12.203 | 1.00 | 57.36 |
| ATOM | 3053 | CD1 | LEU | 595 | 53.375 | -9.692 | 12.533 | 1.00 | 59.51 |
| ATOM | 3054 | CD2 | LEU | 595 | 54.967 | -11.598 | 12.382 | 1.00 | 56.98 |
| ATOM | 3055 | C | LEU | 595 | 51.469 | -14.237 | 13.251 | 1.00 | 56.25 |
| ATOM | 3056 | O | LEU | 595 | 50.314 | -14.359 | 12.834 | 1.00 | 56.60 |
| ATOM | 3057 | N | SER | 596 | 51.927 | -14.845 | 14.341 | 1.00 | 53.07 |
| ATOM | 3058 | CA | SER | 596 | 51.100 | -15.642 | 15.229 | 1.00 | 48.64 |
| ATOM | 3059 | CB | SER | 596 | 51.883 | -16.841 | 15.736 | 1.00 | 46.41 |
| ATOM | 3060 | OG | SER | 596 | 52.806 | -16.435 | 16.737 | 1.00 | 46.50 |
| ATOM | 3061 | C | SER | 596 | 50.796 | -14.756 | 16.423 | 1.00 | 48.95 |
| ATOM | 3062 | O | SER | 596 | 51.492 | -13.767 | 16.649 | 1.00 | 49.39 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3063 | N | SER | 597 | 49.833 | -15.163 | 17.242 | 1.00 | 50.27 |
| ATOM | 3064 | CA | SER | 597 | 49.469 | -14.387 | 18.424 | 1.00 | 51.93 |
| ATOM | 3065 | CB | SER | 597 | 48.391 | -15.123 | 19.225 | 1.00 | 52.03 |
| ATOM | 3066 | OG | SER | 597 | 47.540 | -15.854 | 18.365 | 1.00 | 52.95 |
| ATOM | 3067 | C | SER | 597 | 50.685 | -14.143 | 19.314 | 1.00 | 52.72 |
| ATOM | 3068 | O | SER | 597 | 50.792 | -13.093 | 19.943 | 1.00 | 55.04 |
| ATOM | 3069 | N | LYS | 598 | 51.613 | -15.100 | 19.344 | 1.00 | 53.55 |
| ATOM | 3070 | CA | LYS | 598 | 52.824 | -14.961 | 20.159 | 1.00 | 53.84 |
| ATOM | 3071 | CB | LYS | 598 | 53.566 | -16.295 | 20.248 | 1.00 | 54.25 |
| ATOM | 3072 | CG | LYS | 598 | 54.376 | -16.457 | 21.524 | 1.00 | 57.30 |
| ATOM | 3073 | CD | LYS | 598 | 55.057 | -17.824 | 21.570 | 1.00 | 58.11 |
| ATOM | 3074 | CE | LYS | 598 | 55.780 | -18.055 | 22.893 | 1.00 | 59.00 |
| ATOM | 3075 | NZ | LYS | 598 | 54.840 | -18.169 | 24.043 | 1.00 | 57.85 |
| ATOM | 3076 | C | LYS | 598 | 53.728 | -13.909 | 19.527 | 1.00 | 52.48 |
| ATOM | 3077 | O | LYS | 598 | 54.273 | -13.052 | 20.227 | 1.00 | 51.72 |
| ATOM | 3078 | N | ASP | 599 | 53.842 | -13.960 | 18.198 | 1.00 | 50.65 |
| ATOM | 3079 | CA | ASP | 599 | 54.657 | -13.021 | 17.435 | 1.00 | 48.52 |
| ATOM | 3080 | CB | ASP | 599 | 54.568 | -13.294 | 15.929 | 1.00 | 46.71 |
| ATOM | 3081 | CG | ASP | 599 | 55.233 | -14.607 | 15.515 | 1.00 | 48.88 |
| ATOM | 3082 | OD1 | ASP | 599 | 55.898 | -15.260 | 16.344 | 1.00 | 53.76 |
| ATOM | 3083 | OD2 | ASP | 599 | 55.100 | -14.986 | 14.330 | 1.00 | 46.70 |
| ATOM | 3084 | C | ASP | 599 | 54.173 | -11.598 | 17.706 | 1.00 | 48.66 |
| ATOM | 3085 | O | ASP | 599 | 54.976 | -10.703 | 17.960 | 1.00 | 52.86 |
| ATOM | 3086 | N | LEU | 600 | 52.852 | -11.406 | 17.684 | 1.00 | 44.53 |
| ATOM | 3087 | CA | LEU | 600 | 52.272 | -10.099 | 17.938 | 1.00 | 41.06 |
| ATOM | 3088 | CB | LEU | 600 | 50.774 | -10.100 | 17.632 | 1.00 | 39.23 |
| ATOM | 3089 | CG | LEU | 600 | 50.354 | -10.374 | 16.178 | 1.00 | 36.50 |
| ATOM | 3090 | CD1 | LEU | 600 | 48.850 | -10.272 | 16.063 | 1.00 | 34.99 |
| ATOM | 3091 | CD2 | LEU | 600 | 51.000 | -9.393 | 15.232 | 1.00 | 33.72 |
| ATOM | 3092 | C | LEU | 600 | 52.543 | -9.633 | 19.369 | 1.00 | 40.96 |
| ATOM | 3093 | O | LEU | 600 | 52.890 | -8.467 | 19.580 | 1.00 | 42.04 |
| ATOM | 3094 | N | VAL | 601 | 52.417 | -10.533 | 20.348 | 1.00 | 41.02 |
| ATOM | 3095 | CA | VAL | 601 | 52.685 | -10.156 | 21.744 | 1.00 | 43.57 |
| ATOM | 3096 | CB | VAL | 601 | 52.236 | -11.229 | 22.791 | 1.00 | 43.60 |
| ATOM | 3097 | CG1 | VAL | 601 | 52.254 | -10.607 | 24.205 | 1.00 | 43.44 |
| ATOM | 3098 | CG2 | VAL | 601 | 50.848 | -11.761 | 22.464 | 1.00 | 42.33 |
| ATOM | 3099 | C | VAL | 601 | 54.192 | -9.904 | 21.901 | 1.00 | 42.85 |
| ATOM | 3100 | O | VAL | 601 | 54.611 | -8.989 | 22.611 | 1.00 | 44.28 |
| ATOM | 3101 | N | SER | 602 | 54.986 | -10.685 | 21.175 | 1.00 | 41.33 |
| ATOM | 3102 | CA | SER | 602 | 56.442 | -10.581 | 21.180 | 1.00 | 41.43 |
| ATOM | 3103 | CB | SER | 602 | 57.014 | -11.648 | 20.245 | 1.00 | 40.94 |
| ATOM | 3104 | OG | SER | 602 | 58.434 | -11.612 | 20.184 | 1.00 | 46.26 |
| ATOM | 3105 | C | SER | 602 | 56.859 | -9.176 | 20.722 | 1.00 | 40.58 |
| ATOM | 3106 | O | SER | 602 | 57.629 | -8.497 | 21.403 | 1.00 | 42.32 |
| ATOM | 3107 | N | CYS | 603 | 56.318 | -8.737 | 19.589 | 1.00 | 38.34 |
| ATOM | 3108 | CA | CYS | 603 | 56.580 | -7.409 | 19.051 | 1.00 | 37.28 |
| ATOM | 3109 | CB | CYS | 603 | 55.715 | -7.170 | 17.815 | 1.00 | 38.09 |
| ATOM | 3110 | SG | CYS | 603 | 55.735 | -5.497 | 17.170 | 0.50 | 42.18 |
| ATOM | 3111 | C | CYS | 603 | 56.282 | -6.337 | 20.105 | 1.00 | 35.81 |
| ATOM | 3112 | O | CYS | 603 | 57.038 | -5.380 | 20.241 | 1.00 | 37.87 |
| ATOM | 3113 | N | ALA | 604 | 55.198 | -6.508 | 20.858 | 1.00 | 33.96 |
| ATOM | 3114 | CA | ALA | 604 | 54.804 | -5.572 | 21.911 | 1.00 | 34.97 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3115 | CB | ALA | 604 | 53.393 | -5.917 | 22.409 | 1.00 | 34.13 |
| ATOM | 3116 | C | ALA | 604 | 55.791 | -5.610 | 23.081 | 1.00 | 36.68 |
| ATOM | 3117 | O | ALA | 604 | 56.085 | -4.585 | 23.704 | 1.00 | 36.78 |
| ATOM | 3118 | N | TYR | 605 | 56.281 | -6.807 | 23.385 | 1.00 | 37.68 |
| ATOM | 3119 | CA | TYR | 605 | 57.254 | -7.005 | 24.461 | 1.00 | 38.38 |
| ATOM | 3120 | CB | TYR | 605 | 57.533 | -8.498 | 24.643 | 1.00 | 37.62 |
| ATOM | 3121 | CG | TYR | 605 | 58.635 | -8.806 | 25.622 | 1.00 | 36.56 |
| ATOM | 3122 | CD1 | TYR | 605 | 58.498 | -8.509 | 26.974 | 1.00 | 39.05 |
| ATOM | 3123 | CE1 | TYR | 605 | 59.520 | -8.809 | 27.893 | 1.00 | 41.37 |
| ATOM | 3124 | CD2 | TYR | 605 | 59.812 | -9.407 | 25.198 | 1.00 | 38.09 |
| ATOM | 3125 | CE2 | TYR | 605 | 60.848 | -9.711 | 26.105 | 1.00 | 38.55 |
| ATOM | 3126 | CZ | TYR | 605 | 60.692 | -9.409 | 27.454 | 1.00 | 40.73 |
| ATOM | 3127 | OH | TYR | 605 | 61.707 | -9.704 | 28.348 | 1.00 | 41.44 |
| ATOM | 3128 | C | TYR | 605 | 58.549 | -6.267 | 24.123 | 1.00 | 38.44 |
| ATOM | 3129 | O | TYR | 605 | 59.053 | -5.485 | 24.937 | 1.00 | 40.78 |
| ATOM | 3130 | N | GLN | 606 | 59.053 | -6.501 | 22.908 | 1.00 | 36.07 |
| ATOM | 3131 | CA | GLN | 606 | 60.276 | -5.872 | 22.398 | 1.00 | 35.28 |
| ATOM | 3132 | CB | GLN | 606 | 60.594 | -6.415 | 21.002 | 1.00 | 34.24 |
| ATOM | 3133 | CG | GLN | 606 | 61.105 | -7.851 | 21.005 | 1.00 | 32.26 |
| ATOM | 3134 | CD | GLN | 606 | 61.339 | -8.388 | 19.608 | 1.00 | 30.17 |
| ATOM | 3135 | OE1 | GLN | 606 | 62.274 | -7.988 | 18.907 | 1.00 | 31.89 |
| ATOM | 3136 | NE2 | GLN | 606 | 60.471 | -9.285 | 19.182 | 1.00 | 30.68 |
| ATOM | 3137 | C | GLN | 606 | 60.210 | -4.335 | 22.355 | 1.00 | 36.39 |
| ATOM | 3138 | O | GLN | 606 | 61.206 | -3.660 | 22.632 | 1.00 | 39.59 |
| ATOM | 3139 | N | VAL | 607 | 59.040 | -3.798 | 22.006 | 1.00 | 32.78 |
| ATOM | 3140 | CA | VAL | 607 | 58.839 | -2.350 | 21.944 | 1.00 | 30.29 |
| ATOM | 3141 | CB | VAL | 607 | 57.489 | -1.982 | 21.221 | 1.00 | 28.48 |
| ATOM | 3142 | CG1 | VAL | 607 | 57.219 | -0.488 | 21.298 | 1.00 | 28.68 |
| ATOM | 3143 | CG2 | VAL | 607 | 57.535 | -2.416 | 19.742 | 1.00 | 22.96 |
| ATOM | 3144 | C | VAL | 607 | 58.868 | -1.766 | 23.364 | 1.00 | 30.21 |
| ATOM | 3145 | O | VAL | 607 | 59.469 | -0.705 | 23.591 | 1.00 | 31.24 |
| ATOM | 3146 | N | ALA | 608 | 58.224 | -2.451 | 24.311 | 1.00 | 27.88 |
| ATOM | 3147 | CA | ALA | 608 | 58.187 | -2.001 | 25.694 | 1.00 | 27.66 |
| ATOM | 3148 | CB | ALA | 608 | 57.242 | -2.874 | 26.494 | 1.00 | 26.42 |
| ATOM | 3149 | C | ALA | 608 | 59.585 | -2.019 | 26.309 | 1.00 | 29.04 |
| ATOM | 3150 | O | ALA | 608 | 59.950 | -1.144 | 27.094 | 1.00 | 27.53 |
| ATOM | 3151 | N | ARG | 609 | 60.377 | -3.013 | 25.932 | 1.00 | 28.91 |
| ATOM | 3152 | CA | ARG | 609 | 61.733 | -3.120 | 26.440 | 1.00 | 31.64 |
| ATOM | 3153 | CB | ARG | 609 | 62.394 | -4.405 | 25.953 | 1.00 | 33.78 |
| ATOM | 3154 | CG | ARG | 609 | 61.672 | -5.647 | 26.373 | 1.00 | 38.53 |
| ATOM | 3155 | CD | ARG | 609 | 62.636 | -6.791 | 26.448 | 1.00 | 41.78 |
| ATOM | 3156 | NE | ARG | 609 | 63.319 | -6.838 | 27.733 | 1.00 | 47.58 |
| ATOM | 3157 | CZ | ARG | 609 | 64.441 | -7.510 | 27.955 | 1.00 | 51.52 |
| ATOM | 3158 | NH1 | ARG | 609 | 65.012 | -8.179 | 26.964 | 1.00 | 50.61 |
| ATOM | 3159 | NH2 | ARG | 609 | 64.954 | -7.569 | 29.186 | 1.00 | 54.36 |
| ATOM | 3160 | C | ARG | 609 | 62.581 | -1.918 | 26.024 | 1.00 | 33.26 |
| ATOM | 3161 | O | ARG | 609 | 63.144 | -1.221 | 26.885 | 1.00 | 34.50 |
| ATOM | 3162 | N | GLY | 610 | 62.624 | -1.650 | 24.717 | 1.00 | 30.25 |
| ATOM | 3163 | CA | GLY | 610 | 63.395 | -0.534 | 24.199 | 1.00 | 25.40 |
| ATOM | 3164 | C | GLY | 610 | 63.010 | 0.730 | 24.930 | 1.00 | 24.12 |
| ATOM | 3165 | O | GLY | 610 | 63.857 | 1.507 | 25.345 | 1.00 | 24.74 |
| ATOM | 3166 | N | MET | 611 | 61.712 | 0.907 | 25.131 | 1.00 | 25.81 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3167 | CA | MET | 611 | 61.192 | 2.062 | 25.843 | 1.00 | 26.95 |
| ATOM | 3168 | CB | MET | 611 | 59.672 | 2.121 | 25.702 | 1.00 | 24.60 |
| ATOM | 3169 | CG | MET | 611 | 59.215 | 2.462 | 24.303 | 1.00 | 24.10 |
| ATOM | 3170 | SD | MET | 611 | 59.972 | 4.035 | 23.821 | 1.00 | 26.77 |
| ATOM | 3171 | CE | MET | 611 | 59.546 | 5.090 | 25.184 | 1.00 | 19.21 |
| ATOM | 3172 | C | MET | 611 | 61.600 | 2.071 | 27.314 | 1.00 | 27.68 |
| ATOM | 3173 | O | MET | 611 | 61.891 | 3.128 | 27.865 | 1.00 | 28.22 |
| ATOM | 3174 | N | GLU | 612 | 61.562 | 0.908 | 27.967 | 1.00 | 31.07 |
| ATOM | 3175 | CA | GLU | 612 | 61.955 | 0.791 | 29.382 | 1.00 | 35.25 |
| ATOM | 3176 | CB | GLU | 612 | 61.809 | -0.659 | 29.872 | 1.00 | 34.95 |
| ATOM | 3177 | CG | GLU | 612 | 62.383 | -0.937 | 31.257 | 1.00 | 31.64 |
| ATOM | 3178 | CD | GLU | 612 | 62.392 | -2.422 | 31.631 | 1.00 | 32.34 |
| ATOM | 3179 | OE1 | GLU | 612 | 62.599 | -3.275 | 30.738 | 1.00 | 30.09 |
| ATOM | 3180 | OE2 | GLU | 612 | 62.226 | -2.737 | 32.831 | 1.00 | 33.90 |
| ATOM | 3181 | C | GLU | 612 | 63.409 | 1.252 | 29.468 | 1.00 | 37.14 |
| ATOM | 3182 | O | GLU | 612 | 63.791 | 1.995 | 30.390 | 1.00 | 35.60 |
| ATOM | 3183 | N | TYR | 613 | 64.196 | 0.868 | 28.457 | 1.00 | 37.89 |
| ATOM | 3184 | CA | TYR | 613 | 65.601 | 1.247 | 28.392 | 1.00 | 36.68 |
| ATOM | 3185 | CB | TYR | 613 | 66.328 | 0.531 | 27.246 | 1.00 | 34.23 |
| ATOM | 3186 | CG | TYR | 613 | 67.801 | 0.888 | 27.175 | 1.00 | 36.59 |
| ATOM | 3187 | CD1 | TYR | 613 | 68.734 | 0.263 | 28.005 | 1.00 | 36.83 |
| ATOM | 3188 | CE1 | TYR | 613 | 70.090 | 0.649 | 28.013 | 1.00 | 34.51 |
| ATOM | 3189 | CD2 | TYR | 613 | 68.252 | 1.909 | 26.339 | 1.00 | 35.28 |
| ATOM | 3190 | CE2 | TYR | 613 | 69.596 | 2.306 | 26.340 | 1.00 | 34.09 |
| ATOM | 3191 | CZ | TYR | 613 | 70.512 | 1.674 | 27.181 | 1.00 | 35.91 |
| ATOM | 3192 | OH | TYR | 613 | 71.826 | 2.089 | 27.212 | 1.00 | 29.78 |
| ATOM | 3193 | C | TYR | 613 | 65.724 | 2.760 | 28.233 | 1.00 | 37.58 |
| ATOM | 3194 | O | TYR | 613 | 66.362 | 3.414 | 29.056 | 1.00 | 39.84 |
| ATOM | 3195 | N | LEU | 614 | 65.081 | 3.326 | 27.214 | 1.00 | 35.53 |
| ATOM | 3196 | CA | LEU | 614 | 65.156 | 4.766 | 26.988 | 1.00 | 34.58 |
| ATOM | 3197 | CB | LEU | 614 | 64.314 | 5.157 | 25.781 | 1.00 | 31.88 |
| ATOM | 3198 | CG | LEU | 614 | 64.760 | 4.601 | 24.429 | 1.00 | 29.62 |
| ATOM | 3199 | CD1 | LEU | 614 | 63.783 | 5.016 | 23.346 | 1.00 | 29.19 |
| ATOM | 3200 | CD2 | LEU | 614 | 66.134 | 5.133 | 24.111 | 1.00 | 32.49 |
| ATOM | 3201 | C | LEU | 614 | 64.698 | 5.538 | 28.218 | 1.00 | 36.38 |
| ATOM | 3202 | O | LEU | 614 | 65.325 | 6.525 | 28.618 | 1.00 | 33.81 |
| ATOM | 3203 | N | ALA | 615 | 63.608 | 5.076 | 28.821 | 1.00 | 38.08 |
| ATOM | 3204 | CA | ALA | 615 | 63.066 | 5.711 | 30.018 | 1.00 | 41.01 |
| ATOM | 3205 | CB | ALA | 615 | 61.767 | 5.018 | 30.444 | 1.00 | 42.33 |
| ATOM | 3206 | C | ALA | 615 | 64.099 | 5.683 | 31.147 | 1.00 | 40.47 |
| ATOM | 3207 | O | ALA | 615 | 64.291 | 6.690 | 31.831 | 1.00 | 41.28 |
| ATOM | 3208 | N | SER | 616 | 64.788 | 4.553 | 31.307 | 1.00 | 38.78 |
| ATOM | 3209 | CA | SER | 616 | 65.806 | 4.441 | 32.347 | 1.00 | 40.97 |
| ATOM | 3210 | CB | SER | 616 | 66.354 | 3.009 | 32.454 | 1.00 | 37.82 |
| ATOM | 3211 | OG | SER | 616 | 67.172 | 2.651 | 31.359 | 1.00 | 34.73 |
| ATOM | 3212 | C | SER | 616 | 66.941 | 5.416 | 32.061 | 1.00 | 42.68 |
| ATOM | 3213 | O | SER | 616 | 67.714 | 5.769 | 32.957 | 1.00 | 45.78 |
| ATOM | 3214 | N | LYS | 617 | 67.015 | 5.869 | 30.815 | 1.00 | 40.92 |
| ATOM | 3215 | CA | LYS | 617 | 68.025 | 6.816 | 30.380 | 1.00 | 38.04 |
| ATOM | 3216 | CB | LYS | 617 | 68.541 | 6.411 | 29.003 | 1.00 | 38.25 |
| ATOM | 3217 | CG | LYS | 617 | 69.293 | 5.111 | 29.021 | 1.00 | 36.40 |
| ATOM | 3218 | CD | LYS | 617 | 70.421 | 5.221 | 29.992 | 1.00 | 38.14 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3219 | CE | LYS | 617 | 71.215 | 3.941 | 30.086 | 1.00 | 38.43 |
| ATOM | 3220 | NZ | LYS | 617 | 72.530 | 4.210 | 30.751 | 1.00 | 43.07 |
| ATOM | 3221 | C | LYS | 617 | 67.475 | 8.242 | 30.350 | 1.00 | 38.42 |
| ATOM | 3222 | O | LYS | 617 | 68.072 | 9.133 | 29.744 | 1.00 | 41.37 |
| ATOM | 3223 | N | LYS | 618 | 66.323 | 8.444 | 30.985 | 1.00 | 37.25 |
| ATOM | 3224 | CA | LYS | 618 | 65.674 | 9.743 | 31.067 | 1.00 | 36.75 |
| ATOM | 3225 | CB | LYS | 618 | 66.653 | 10.780 | 31.632 | 1.00 | 43.27 |
| ATOM | 3226 | CG | LYS | 618 | 67.340 | 10.392 | 32.938 | 1.00 | 51.59 |
| ATOM | 3227 | CD | LYS | 618 | 66.377 | 10.361 | 34.092 | 1.00 | 61.24 |
| ATOM | 3228 | CE | LYS | 618 | 67.070 | 9.945 | 35.373 | 1.00 | 67.83 |
| ATOM | 3229 | NZ | LYS | 618 | 66.105 | 10.039 | 36.510 | 1.00 | 75.22 |
| ATOM | 3230 | C | LYS | 618 | 65.167 | 10.222 | 29.706 | 1.00 | 36.61 |
| ATOM | 3231 | O | LYS | 618 | 64.856 | 11.396 | 29.535 | 1.00 | 35.94 |
| ATOM | 3232 | N | CYS | 619 | 65.058 | 9.308 | 28.751 | 1.00 | 36.26 |
| ATOM | 3233 | CA | CYS | 619 | 64.603 | 9.666 | 27.412 | 1.00 | 33.41 |
| ATOM | 3234 | CB | CYS | 619 | 65.351 | 8.843 | 26.365 | 1.00 | 32.17 |
| ATOM | 3235 | SG | CYS | 619 | 65.006 | 9.223 | 24.650 | 1.00 | 26.92 |
| ATOM | 3236 | C | CYS | 619 | 63.108 | 9.546 | 27.194 | 1.00 | 32.29 |
| ATOM | 3237 | O | CYS | 619 | 62.510 | 8.472 | 27.373 | 1.00 | 29.13 |
| ATOM | 3238 | N | ILE | 620 | 62.515 | 10.679 | 26.827 | 1.00 | 31.60 |
| ATOM | 3239 | CA | ILE | 620 | 61.091 | 10.763 | 26.528 | 1.00 | 31.21 |
| ATOM | 3240 | CB | ILE | 620 | 60.435 | 11.966 | 27.212 | 1.00 | 29.57 |
| ATOM | 3241 | CG2 | ILE | 620 | 58.955 | 12.031 | 26.860 | 1.00 | 31.49 |
| ATOM | 3242 | CG1 | ILE | 620 | 60.578 | 11.848 | 28.727 | 1.00 | 27.85 |
| ATOM | 3243 | CD1 | ILE | 620 | 60.065 | 13.046 | 29.463 | 1.00 | 26.50 |
| ATOM | 3244 | C | ILE | 620 | 61.034 | 10.972 | 25.018 | 1.00 | 32.18 |
| ATOM | 3245 | O | ILE | 620 | 61.481 | 11.993 | 24.512 | 1.00 | 33.18 |
| ATOM | 3246 | N | HIS | 621 | 60.472 | 9.990 | 24.318 | 1.00 | 31.93 |
| ATOM | 3247 | CA | HIS | 621 | 60.354 | 9.970 | 22.864 | 1.00 | 32.59 |
| ATOM | 3248 | CB | HIS | 621 | 59.933 | 8.552 | 22.420 | 1.00 | 29.51 |
| ATOM | 3249 | CG | HIS | 621 | 60.076 | 8.288 | 20.951 | 1.00 | 27.45 |
| ATOM | 3250 | CD2 | HIS | 621 | 60.663 | 7.262 | 20.286 | 1.00 | 25.84 |
| ATOM | 3251 | ND1 | HIS | 621 | 59.528 | 9.106 | 19.979 | 1.00 | 25.20 |
| ATOM | 3252 | CE1 | HIS | 621 | 59.774 | 8.596 | 18.783 | 1.00 | 25.07 |
| ATOM | 3253 | NE2 | HIS | 621 | 60.456 | 7.473 | 18.942 | 1.00 | 23.24 |
| ATOM | 3254 | C | HIS | 621 | 59.365 | 10.992 | 22.320 | 1.00 | 35.31 |
| ATOM | 3255 | O | HIS | 621 | 59.555 | 11.481 | 21.220 | 1.00 | 39.24 |
| ATOM | 3256 | N | ARG | 622 | 58.256 | 11.216 | 23.028 | 1.00 | 36.50 |
| ATOM | 3257 | CA | ARG | 622 | 57.225 | 12.169 | 22.580 | 1.00 | 35.78 |
| ATOM | 3258 | CB | ARG | 622 | 57.783 | 13.582 | 22.462 | 1.00 | 32.55 |
| ATOM | 3259 | CG | ARG | 622 | 58.211 | 14.156 | 23.778 | 1.00 | 30.54 |
| ATOM | 3260 | CD | ARG | 622 | 58.799 | 15.551 | 23.635 | 0.50 | 27.28 |
| ATOM | 3261 | NE | ARG | 622 | 59.249 | 16.043 | 24.930 | 0.50 | 24.53 |
| ATOM | 3262 | CZ | ARG | 622 | 60.409 | 15.707 | 25.499 | 0.50 | 27.85 |
| ATOM | 3263 | NH1 | ARG | 622 | 61.249 | 14.883 | 24.877 | 0.50 | 27.61 |
| ATOM | 3264 | NH2 | ARG | 622 | 60.711 | 16.158 | 26.714 | 0.50 | 25.34 |
| ATOM | 3265 | C | ARG | 622 | 56.447 | 11.806 | 21.297 | 1.00 | 35.76 |
| ATOM | 3266 | O | ARG | 622 | 55.438 | 12.430 | 20.999 | 1.00 | 36.61 |
| ATOM | 3267 | N | ASP | 623 | 56.923 | 10.818 | 20.537 | 1.00 | 34.69 |
| ATOM | 3268 | CA | ASP | 623 | 56.197 | 10.400 | 19.335 | 1.00 | 34.09 |
| ATOM | 3269 | CB | ASP | 623 | 56.628 | 11.171 | 18.081 | 1.00 | 34.77 |
| ATOM | 3270 | CG | ASP | 623 | 55.727 | 10.869 | 16.863 | 1.00 | 43.51 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3271 | OD1 | ASP | 623 | 56.213 | 10.992 | 15.714 | 1.00 | 47.45 |
| ATOM | 3272 | OD2 | ASP | 623 | 54.538 | 10.509 | 17.032 | 1.00 | 47.51 |
| ATOM | 3273 | C | ASP | 623 | 56.321 | 8.903 | 19.115 | 1.00 | 32.51 |
| ATOM | 3274 | O | ASP | 623 | 56.635 | 8.435 | 18.025 | 1.00 | 31.80 |
| ATOM | 3275 | N | LEU | 624 | 56.081 | 8.135 | 20.164 | 1.00 | 31.80 |
| ATOM | 3276 | CA | LEU | 624 | 56.152 | 6.689 | 20.030 | 1.00 | 31.07 |
| ATOM | 3277 | CB | LEU | 624 | 56.133 | 6.029 | 21.403 | 1.00 | 28.11 |
| ATOM | 3278 | CG | LEU | 624 | 55.983 | 4.510 | 21.460 | 1.00 | 27.88 |
| ATOM | 3279 | CD1 | LEU | 624 | 57.108 | 3.809 | 20.700 | 1.00 | 23.96 |
| ATOM | 3280 | CD2 | LEU | 624 | 56.001 | 4.088 | 22.912 | 1.00 | 29.50 |
| ATOM | 3281 | C | LEU | 624 | 54.954 | 6.238 | 19.187 | 1.00 | 32.04 |
| ATOM | 3282 | O | LEU | 624 | 53.805 | 6.564 | 19.505 | 1.00 | 36.02 |
| ATOM | 3283 | N | ALA | 625 | 55.224 | 5.561 | 18.076 | 1.00 | 28.91 |
| ATOM | 3284 | CA | ALA | 625 | 54.170 | 5.066 | 17.192 | 1.00 | 25.66 |
| ATOM | 3285 | CB | ALA | 625 | 53.707 | 6.170 | 16.289 | 1.00 | 23.37 |
| ATOM | 3286 | C | ALA | 625 | 54.800 | 3.948 | 16.389 | 1.00 | 27.71 |
| ATOM | 3287 | O | ALA | 625 | 56.022 | 3.841 | 16.355 | 1.00 | 29.77 |
| ATOM | 3288 | N | ALA | 626 | 53.982 | 3.107 | 15.758 | 1.00 | 29.46 |
| ATOM | 3289 | CA | ALA | 626 | 54.499 | 1.993 | 14.956 | 1.00 | 28.16 |
| ATOM | 3290 | CB | ALA | 626 | 53.350 | 1.155 | 14.401 | 1.00 | 28.02 |
| ATOM | 3291 | C | ALA | 626 | 55.366 | 2.504 | 13.831 | 1.00 | 26.78 |
| ATOM | 3292 | O | ALA | 626 | 56.329 | 1.859 | 13.454 | 1.00 | 26.69 |
| ATOM | 3293 | N | ARG | 627 | 55.022 | 3.680 | 13.314 | 1.00 | 26.09 |
| ATOM | 3294 | CA | ARG | 627 | 55.777 | 4.301 | 12.246 | 1.00 | 26.78 |
| ATOM | 3295 | CB | ARG | 627 | 55.134 | 5.637 | 11.837 | 1.00 | 27.01 |
| ATOM | 3296 | CG | ARG | 627 | 55.046 | 6.672 | 12.961 | 1.00 | 29.34 |
| ATOM | 3297 | CD | ARG | 627 | 54.552 | 8.037 | 12.477 | 1.00 | 34.26 |
| ATOM | 3298 | NE | ARG | 627 | 54.108 | 8.878 | 13.590 | 1.00 | 36.96 |
| ATOM | 3299 | CZ | ARG | 627 | 52.867 | 8.889 | 14.059 | 1.00 | 40.84 |
| ATOM | 3300 | NH1 | ARG | 627 | 51.942 | 8.114 | 13.515 | 1.00 | 42.56 |
| ATOM | 3301 | NH2 | ARG | 627 | 52.552 | 9.634 | 15.108 | 1.00 | 45.20 |
| ATOM | 3302 | C | ARG | 627 | 57.209 | 4.549 | 12.711 | 1.00 | 29.11 |
| ATOM | 3303 | O | ARG | 627 | 58.137 | 4.468 | 11.911 | 1.00 | 30.39 |
| ATOM | 3304 | N | ASN | 628 | 57.385 | 4.804 | 14.010 | 1.00 | 30.37 |
| ATOM | 3305 | CA | ASN | 628 | 58.689 | 5.092 | 14.596 | 1.00 | 27.02 |
| ATOM | 3306 | CB | ASN | 628 | 58.578 | 6.226 | 15.611 | 1.00 | 24.35 |
| ATOM | 3307 | CG | ASN | 628 | 58.383 | 7.571 | 14.941 | 1.00 | 25.95 |
| ATOM | 3308 | OD1 | ASN | 628 | 58.992 | 7.865 | 13.924 | 1.00 | 32.01 |
| ATOM | 3309 | ND2 | ASN | 628 | 57.522 | 8.391 | 15.503 | 1.00 | 24.34 |
| ATOM | 3310 | C | ASN | 628 | 59.437 | 3.903 | 15.185 | 1.00 | 26.74 |
| ATOM | 3311 | O | ASN | 628 | 60.378 | 4.062 | 15.972 | 1.00 | 28.49 |
| ATOM | 3312 | N | VAL | 629 | 58.998 | 2.712 | 14.802 | 1.00 | 27.34 |
| ATOM | 3313 | CA | VAL | 629 | 59.621 | 1.450 | 15.224 | 1.00 | 24.94 |
| ATOM | 3314 | CB | VAL | 629 | 58.589 | 0.522 | 15.906 | 1.00 | 22.20 |
| ATOM | 3315 | CG1 | VAL | 629 | 59.169 | -0.883 | 16.089 | 1.00 | 18.03 |
| ATOM | 3316 | CG2 | VAL | 629 | 58.158 | 1.121 | 17.244 | 1.00 | 18.34 |
| ATOM | 3317 | C | VAL | 629 | 60.077 | 0.805 | 13.918 | 1.00 | 26.84 |
| ATOM | 3318 | O | VAL | 629 | 59.284 | 0.679 | 12.978 | 1.00 | 26.50 |
| ATOM | 3319 | N | LEU | 630 | 61.352 | 0.469 | 13.809 | 1.00 | 27.66 |
| ATOM | 3320 | CA | LEU | 630 | 61.862 | -0.158 | 12.601 | 1.00 | 30.14 |
| ATOM | 3321 | CB | LEU | 630 | 63.105 | 0.577 | 12.122 | 1.00 | 28.00 |
| ATOM | 3322 | CG | LEU | 630 | 62.856 | 2.086 | 12.027 | 1.00 | 26.06 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3323 | CD1 | LEU | 630 | 64.150 | 2.831 | 11.832 | 1.00 | 23.44 |
| ATOM | 3324 | CD2 | LEU | 630 | 61.880 | 2.381 | 10.901 | 1.00 | 27.72 |
| ATOM | 3325 | C | LEU | 630 | 62.145 | -1.627 | 12.889 | 1.00 | 32.90 |
| ATOM | 3326 | O | LEU | 630 | 62.437 | -1.982 | 14.029 | 1.00 | 33.06 |
| ATOM | 3327 | N | VAL | 631 | 61.991 | -2.478 | 11.873 | 1.00 | 34.83 |
| ATOM | 3328 | CA | VAL | 631 | 62.195 | -3.928 | 12.006 | 1.00 | 33.02 |
| ATOM | 3329 | CB | VAL | 631 | 60.915 | -4.700 | 11.584 | 1.00 | 30.92 |
| ATOM | 3330 | CG1 | VAL | 631 | 61.071 | -6.208 | 11.842 | 1.00 | 27.66 |
| ATOM | 3331 | CG2 | VAL | 631 | 59.724 | -4.161 | 12.332 | 1.00 | 24.46 |
| ATOM | 3332 | C | VAL | 631 | 63.371 | -4.415 | 11.161 | 1.00 | 35.77 |
| ATOM | 3333 | O | VAL | 631 | 63.428 | -4.171 | 9.954 | 1.00 | 37.57 |
| ATOM | 3334 | N | THR | 632 | 64.319 | -5.098 | 11.797 | 1.00 | 37.96 |
| ATOM | 3335 | CA | THR | 632 | 65.511 | -5.599 | 11.096 | 1.00 | 39.06 |
| ATOM | 3336 | CB | THR | 632 | 66.675 | -5.820 | 12.066 | 1.00 | 35.55 |
| ATOM | 3337 | OG1 | THR | 632 | 66.368 | -6.903 | 12.955 | 1.00 | 35.76 |
| ATOM | 3338 | CG2 | THR | 632 | 66.928 | -4.561 | 12.867 | 1.00 | 35.06 |
| ATOM | 3339 | C | THR | 632 | 65.283 | -6.893 | 10.331 | 1.00 | 40.66 |
| ATOM | 3340 | O | THR | 632 | 64.238 | -7.515 | 10.466 | 1.00 | 41.79 |
| ATOM | 3341 | N | GLU | 633 | 66.282 | -7.307 | 9.556 | 1.00 | 43.40 |
| ATOM | 3342 | CA | GLU | 633 | 66.219 | -8.540 | 8.768 | 1.00 | 45.33 |
| ATOM | 3343 | CB | GLU | 633 | 67.501 | -8.689 | 7.942 | 1.00 | 48.67 |
| ATOM | 3344 | CG | GLU | 633 | 67.496 | -9.791 | 6.864 | 1.00 | 54.70 |
| ATOM | 3345 | CD | GLU | 633 | 66.599 | -9.506 | 5.647 | 1.00 | 58.16 |
| ATOM | 3346 | OE1 | GLU | 633 | 65.933 | -8.452 | 5.567 | 1.00 | 60.68 |
| ATOM | 3347 | OE2 | GLU | 633 | 66.566 | -10.369 | 4.747 | 1.00 | 60.14 |
| ATOM | 3348 | C | GLU | 633 | 66.011 | -9.774 | 9.648 | 1.00 | 46.02 |
| ATOM | 3349 | O | GLU | 633 | 65.637 | -10.834 | 9.156 | 1.00 | 46.75 |
| ATOM | 3350 | N | ASP | 634 | 66.278 | -9.648 | 10.944 | 1.00 | 46.45 |
| ATOM | 3351 | CA | ASP | 634 | 66.085 | -10.774 | 11.843 | 1.00 | 46.14 |
| ATOM | 3352 | CB | ASP | 634 | 67.316 | -10.995 | 12.724 | 1.00 | 52.89 |
| ATOM | 3353 | CG | ASP | 634 | 68.570 | -11.399 | 11.929 | 1.00 | 59.65 |
| ATOM | 3354 | OD1 | ASP | 634 | 68.593 | -12.499 | 11.328 | 1.00 | 59.91 |
| ATOM | 3355 | OD2 | ASP | 634 | 69.546 | -10.608 | 11.918 | 1.00 | 62.29 |
| ATOM | 3356 | C | ASP | 634 | 64.850 | -10.549 | 12.708 | 1.00 | 45.75 |
| ATOM | 3357 | O | ASP | 634 | 64.729 | -11.138 | 13.776 | 1.00 | 46.38 |
| ATOM | 3358 | N | ASN | 635 | 63.940 | -9.697 | 12.235 | 1.00 | 45.92 |
| ATOM | 3359 | CA | ASN | 635 | 62.690 | -9.367 | 12.915 | 1.00 | 44.36 |
| ATOM | 3360 | CB | ASN | 635 | 61.750 | -10.583 | 12.972 | 1.00 | 46.62 |
| ATOM | 3361 | CG | ASN | 635 | 61.409 | -11.116 | 11.597 | 1.00 | 47.56 |
| ATOM | 3362 | OD1 | ASN | 635 | 60.750 | -10.453 | 10.800 | 1.00 | 50.54 |
| ATOM | 3363 | ND2 | ASN | 635 | 61.876 | -12.314 | 11.305 | 1.00 | 47.75 |
| ATOM | 3364 | C | ASN | 635 | 62.833 | -8.763 | 14.308 | 1.00 | 42.78 |
| ATOM | 3365 | O | ASN | 635 | 62.028 | -9.045 | 15.189 | 1.00 | 44.56 |
| ATOM | 3366 | N | VAL | 636 | 63.849 | -7.927 | 14.503 | 1.00 | 41.03 |
| ATOM | 3367 | CA | VAL | 636 | 64.071 | -7.291 | 15.797 | 1.00 | 36.87 |
| ATOM | 3368 | CB | VAL | 636 | 65.584 | -7.162 | 16.083 | 1.00 | 35.99 |
| ATOM | 3369 | CG1 | VAL | 636 | 65.839 | -6.347 | 17.354 | 1.00 | 34.01 |
| ATOM | 3370 | CG2 | VAL | 636 | 66.184 | -8.535 | 16.226 | 1.00 | 33.65 |
| ATOM | 3371 | C | VAL | 636 | 63.434 | -5.908 | 15.782 | 1.00 | 34.79 |
| ATOM | 3372 | O | VAL | 636 | 63.657 | -5.131 | 14.854 | 1.00 | 36.58 |
| ATOM | 3373 | N | MET | 637 | 62.600 | -5.625 | 16.773 | 1.00 | 32.04 |
| ATOM | 3374 | CA | MET | 637 | 61.940 | -4.331 | 16.887 | 1.00 | 31.14 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3375 | CB | MET | 637 | 60.734 | -4.427 | 17.817 | 1.00 | 35.49 |
| ATOM | 3376 | CG | MET | 637 | 59.702 | -5.501 | 17.437 | 1.00 | 37.77 |
| ATOM | 3377 | SD | MET | 637 | 58.835 | -5.257 | 15.857 | 1.00 | 39.62 |
| ATOM | 3378 | CE | MET | 637 | 59.122 | -6.864 | 15.035 | 1.00 | 34.87 |
| ATOM | 3379 | C | MET | 637 | 62.935 | -3.342 | 17.479 | 1.00 | 29.95 |
| ATOM | 3380 | O | MET | 637 | 63.525 | -3.612 | 18.526 | 1.00 | 26.48 |
| ATOM | 3381 | N | LYS | 638 | 63.044 | -2.167 | 16.861 | 1.00 | 29.03 |
| ATOM | 3382 | CA | LYS | 638 | 63.977 | -1.133 | 17.293 | 1.00 | 24.64 |
| ATOM | 3383 | CB | LYS | 638 | 65.214 | -1.150 | 16.390 | 1.00 | 22.85 |
| ATOM | 3384 | CG | LYS | 638 | 66.145 | -2.305 | 16.655 | 1.00 | 17.56 |
| ATOM | 3385 | CD | LYS | 638 | 67.307 | -2.274 | 15.707 | 1.00 | 19.48 |
| ATOM | 3386 | CE | LYS | 638 | 68.369 | -3.242 | 16.146 | 1.00 | 17.71 |
| ATOM | 3387 | NZ | LYS | 638 | 68.931 | -2.895 | 17.473 | 1.00 | 24.81 |
| ATOM | 3388 | C | LYS | 638 | 63.367 | 0.260 | 17.270 | 1.00 | 24.75 |
| ATOM | 3389 | O | LYS | 638 | 62.987 | 0.740 | 16.203 | 1.00 | 24.35 |
| ATOM | 3390 | N | ILE | 639 | 63.277 | 0.905 | 18.437 | 1.00 | 24.63 |
| ATOM | 3391 | CA | ILE | 639 | 62.734 | 2.256 | 18.536 | 1.00 | 24.75 |
| ATOM | 3392 | CB | ILE | 639 | 62.699 | 2.789 | 19.993 | 1.00 | 23.98 |
| ATOM | 3393 | CG2 | ILE | 639 | 61.916 | 4.094 | 20.046 | 1.00 | 21.11 |
| ATOM | 3394 | CG1 | ILE | 639 | 62.127 | 1.740 | 20.963 | 1.00 | 26.06 |
| ATOM | 3395 | CD1 | ILE | 639 | 60.680 | 1.392 | 20.758 | 1.00 | 28.45 |
| ATOM | 3396 | C | ILE | 639 | 63.656 | 3.198 | 17.774 | 1.00 | 26.36 |
| ATOM | 3397 | O | ILE | 639 | 64.884 | 3.161 | 17.947 | 1.00 | 25.06 |
| ATOM | 3398 | N | ALA | 640 | 63.073 | 4.072 | 16.963 | 1.00 | 26.70 |
| ATOM | 3399 | CA | ALA | 640 | 63.857 | 5.037 | 16.202 | 1.00 | 27.85 |
| ATOM | 3400 | CB | ALA | 640 | 63.683 | 4.777 | 14.736 | 1.00 | 27.66 |
| ATOM | 3401 | C | ALA | 640 | 63.380 | 6.449 | 16.548 | 1.00 | 29.56 |
| ATOM | 3402 | O | ALA | 640 | 62.307 | 6.608 | 17.136 | 1.00 | 29.82 |
| ATOM | 3403 | N | ASP | 641 | 64.174 | 7.456 | 16.180 | 1.00 | 28.74 |
| ATOM | 3404 | CA | ASP | 641 | 63.863 | 8.874 | 16.415 | 1.00 | 32.13 |
| ATOM | 3405 | CB | ASP | 641 | 62.662 | 9.310 | 15.574 | 1.00 | 35.25 |
| ATOM | 3406 | CG | ASP | 641 | 63.024 | 9.555 | 14.121 | 1.00 | 38.54 |
| ATOM | 3407 | OD1 | ASP | 641 | 64.149 | 9.170 | 13.716 | 1.00 | 39.85 |
| ATOM | 3408 | OD2 | ASP | 641 | 62.192 | 10.144 | 13.394 | 1.00 | 41.38 |
| ATOM | 3409 | C | ASP | 641 | 63.661 | 9.311 | 17.862 | 1.00 | 30.61 |
| ATOM | 3410 | O | ASP | 641 | 63.012 | 10.323 | 18.140 | 1.00 | 29.45 |
| ATOM | 3411 | N | PHE | 642 | 64.265 | 8.567 | 18.776 | 1.00 | 30.96 |
| ATOM | 3412 | CA | PHE | 642 | 64.155 | 8.860 | 20.195 | 1.00 | 31.21 |
| ATOM | 3413 | CB | PHE | 642 | 64.447 | 7.597 | 21.013 | 1.00 | 27.06 |
| ATOM | 3414 | CG | PHE | 642 | 65.806 | 7.008 | 20.749 | 1.00 | 24.27 |
| ATOM | 3415 | CD1 | PHE | 642 | 66.930 | 7.476 | 21.419 | 1.00 | 22.36 |
| ATOM | 3416 | CD2 | PHE | 642 | 65.962 | 5.978 | 19.838 | 1.00 | 24.87 |
| ATOM | 3417 | CE1 | PHE | 642 | 68.179 | 6.928 | 21.190 | 1.00 | 23.19 |
| ATOM | 3418 | CE2 | PHE | 642 | 67.205 | 5.420 | 19.603 | 1.00 | 23.65 |
| ATOM | 3419 | CZ | PHE | 642 | 68.323 | 5.898 | 20.282 | 1.00 | 22.95 |
| ATOM | 3420 | C | PHE | 642 | 65.069 | 10.007 | 20.623 | 1.00 | 34.88 |
| ATOM | 3421 | O | PHE | 642 | 64.920 | 10.549 | 21.729 | 1.00 | 34.84 |
| ATOM | 3422 | N | GLY | 643 | 66.000 | 10.377 | 19.737 | 1.00 | 36.20 |
| ATOM | 3423 | CA | GLY | 643 | 66.934 | 11.450 | 20.032 | 1.00 | 35.47 |
| ATOM | 3424 | C | GLY | 643 | 66.728 | 12.720 | 19.232 | 1.00 | 37.62 |
| ATOM | 3425 | O | GLY | 643 | 67.581 | 13.593 | 19.269 | 1.00 | 39.16 |
| ATOM | 3426 | N | LEU | 644 | 65.609 | 12.837 | 18.517 | 1.00 | 39.68 |

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ATOM    3427  CA  LEU   644       65.328  14.029  17.712  1.00 43.09
ATOM    3428  CB  LEU   644       64.074  13.843  16.860  1.00 40.78
ATOM    3429  CG  LEU   644       64.076  12.876  15.681  1.00 36.94
ATOM    3430  CD1 LEU   644       62.790  13.076  14.901  1.00 37.34
ATOM    3431  CD2 LEU   644       65.240  13.157  14.783  1.00 37.72
ATOM    3432  C   LEU   644       65.154  15.261  18.591  1.00 47.32
ATOM    3433  O   LEU   644       64.639  15.170  19.702  1.00 50.33
ATOM    3434  N   ALA   645       65.598  16.406  18.088  1.00 51.23
ATOM    3435  CA  ALA   645       65.507  17.662  18.820  1.00 52.97
ATOM    3436  CB  ALA   645       66.367  18.703  18.151  1.00 54.12
ATOM    3437  C   ALA   645       64.060  18.137  18.910  1.00 53.00
ATOM    3438  O   ALA   645       63.591  18.528  19.977  1.00 53.59
ATOM    3439  N   ASP   652       52.356  21.675  14.855  1.00 79.51
ATOM    3440  CA  ASP   652       51.194  21.821  13.993  1.00 78.74
ATOM    3441  CB  ASP   652       51.625  22.021  12.531  1.00 78.30
ATOM    3442  CG  ASP   652       50.459  22.358  11.608  1.00 77.64
ATOM    3443  OD1 ASP   652       49.473  22.968  12.079  1.00 77.67
ATOM    3444  OD2 ASP   652       50.526  22.029  10.410  1.00 78.25
ATOM    3445  C   ASP   652       50.339  20.569  14.125  1.00 78.92
ATOM    3446  O   ASP   652       50.645  19.529  13.539  1.00 79.36
ATOM    3447  N   TYR   653       49.262  20.682  14.892  1.00 79.17
ATOM    3448  CA  TYR   653       48.357  19.560  15.111  1.00 80.23
ATOM    3449  CB  TYR   653       47.283  19.932  16.136  1.00 81.36
ATOM    3450  CG  TYR   653       47.790  20.060  17.557  1.00 84.51
ATOM    3451  CD1 TYR   653       46.998  20.649  18.544  1.00 86.09
ATOM    3452  CE1 TYR   653       47.443  20.751  19.865  1.00 88.05
ATOM    3453  CD2 TYR   653       49.049  19.576  17.925  1.00 86.22
ATOM    3454  CE2 TYR   653       49.504  19.673  19.242  1.00 87.14
ATOM    3455  CZ  TYR   653       48.698  20.260  20.207  1.00 88.37
ATOM    3456  OH  TYR   653       49.146  20.351  21.510  1.00 88.82
ATOM    3457  C   TYR   653       47.687  19.098  13.827  1.00 80.07
ATOM    3458  O   TYR   653       47.170  17.983  13.752  1.00 81.23
ATOM    3459  N   TYR   654       47.716  19.953  12.813  1.00 79.01
ATOM    3460  CA  TYR   654       47.082  19.640  11.544  1.00 78.81
ATOM    3461  CB  TYR   654       46.378  20.884  11.008  1.00 78.48
ATOM    3462  CG  TYR   654       45.358  21.422  11.982  1.00 78.53
ATOM    3463  CD1 TYR   654       45.752  21.948  13.213  1.00 77.46
ATOM    3464  CE1 TYR   654       44.822  22.382  14.146  1.00 78.94
ATOM    3465  CD2 TYR   654       43.997  21.350  11.704  1.00 80.18
ATOM    3466  CE2 TYR   654       43.054  21.785  12.632  1.00 82.55
ATOM    3467  CZ  TYR   654       43.473  22.297  13.851  1.00 80.98
ATOM    3468  OH  TYR   654       42.548  22.703  14.785  1.00 82.29
ATOM    3469  C   TYR   654       48.010  19.042  10.499  1.00 79.04
ATOM    3470  O   TYR   654       47.575  18.720   9.393  1.00 80.09
ATOM    3471  N   LYS   655       49.277  18.859  10.848  1.00 78.74
ATOM    3472  CA  LYS   655       50.217  18.282   9.906  1.00 80.69
ATOM    3473  CB  LYS   655       51.651  18.687  10.247  1.00 83.97
ATOM    3474  CG  LYS   655       52.674  18.124   9.281  1.00 89.76
ATOM    3475  CD  LYS   655       54.084  18.565   9.611  1.00 93.90
ATOM    3476  CE  LYS   655       55.075  17.844   8.708  1.00 97.62
ATOM    3477  NZ  LYS   655       56.489  18.177   9.038  1.00101.35
ATOM    3478  C   LYS   655       50.070  16.763   9.922  1.00 80.98
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3479 | O | LYS | 655 | 50.187 | 16.130 | 10.975 | 1.00 | 80.95 |
| ATOM | 3480 | N | LYS | 656 | 49.766 | 16.194 | 8.759 | 1.00 | 81.29 |
| ATOM | 3481 | CA | LYS | 656 | 49.599 | 14.749 | 8.630 | 1.00 | 81.06 |
| ATOM | 3482 | CB | LYS | 656 | 48.723 | 14.426 | 7.423 | 1.00 | 81.40 |
| ATOM | 3483 | CG | LYS | 656 | 47.258 | 14.779 | 7.596 | 1.00 | 81.60 |
| ATOM | 3484 | CD | LYS | 656 | 46.518 | 14.565 | 6.295 | 1.00 | 84.93 |
| ATOM | 3485 | CE | LYS | 656 | 45.019 | 14.620 | 6.493 | 1.00 | 87.78 |
| ATOM | 3486 | NZ | LYS | 656 | 44.291 | 14.565 | 5.183 | 1.00 | 91.78 |
| ATOM | 3487 | C | LYS | 656 | 50.940 | 14.026 | 8.513 | 1.00 | 80.44 |
| ATOM | 3488 | O | LYS | 656 | 51.923 | 14.596 | 8.032 | 1.00 | 80.35 |
| ATOM | 3489 | N | GLY | 660 | 49.197 | 9.779 | 5.831 | 1.00 | 57.41 |
| ATOM | 3490 | CA | GLY | 660 | 48.231 | 10.860 | 5.961 | 1.00 | 55.59 |
| ATOM | 3491 | C | GLY | 660 | 47.492 | 10.866 | 7.285 | 1.00 | 53.27 |
| ATOM | 3492 | O | GLY | 660 | 46.403 | 11.432 | 7.388 | 1.00 | 53.03 |
| ATOM | 3493 | N | ARG | 661 | 48.080 | 10.222 | 8.288 | 1.00 | 51.92 |
| ATOM | 3494 | CA | ARG | 661 | 47.477 | 10.155 | 9.617 | 1.00 | 48.40 |
| ATOM | 3495 | CB | ARG | 661 | 47.900 | 8.861 | 10.338 | 1.00 | 50.20 |
| ATOM | 3496 | CG | ARG | 661 | 47.612 | 7.566 | 9.563 | 1.00 | 49.76 |
| ATOM | 3497 | CD | ARG | 661 | 47.801 | 6.331 | 10.456 | 1.00 | 52.48 |
| ATOM | 3498 | NE | ARG | 661 | 47.691 | 5.061 | 9.734 | 1.00 | 52.60 |
| ATOM | 3499 | CZ | ARG | 661 | 47.955 | 3.866 | 10.264 | 1.00 | 50.93 |
| ATOM | 3500 | NH1 | ARG | 661 | 48.343 | 3.760 | 11.529 | 1.00 | 48.54 |
| ATOM | 3501 | NH2 | ARG | 661 | 47.836 | 2.772 | 9.523 | 1.00 | 52.75 |
| ATOM | 3502 | C | ARG | 661 | 47.894 | 11.379 | 10.439 | 1.00 | 43.81 |
| ATOM | 3503 | O | ARG | 661 | 48.833 | 12.096 | 10.063 | 1.00 | 43.23 |
| ATOM | 3504 | N | LEU | 662 | 47.194 | 11.618 | 11.537 | 1.00 | 40.56 |
| ATOM | 3505 | CA | LEU | 662 | 47.496 | 12.735 | 12.428 | 1.00 | 37.52 |
| ATOM | 3506 | CB | LEU | 662 | 46.220 | 13.496 | 12.789 | 1.00 | 33.26 |
| ATOM | 3507 | CG | LEU | 662 | 45.485 | 14.281 | 11.696 | 1.00 | 31.29 |
| ATOM | 3508 | CD1 | LEU | 662 | 44.084 | 14.621 | 12.158 | 1.00 | 24.03 |
| ATOM | 3509 | CD2 | LEU | 662 | 46.261 | 15.535 | 11.358 | 1.00 | 28.65 |
| ATOM | 3510 | C | LEU | 662 | 48.154 | 12.237 | 13.712 | 1.00 | 36.78 |
| ATOM | 3511 | O | LEU | 662 | 47.515 | 11.570 | 14.536 | 1.00 | 37.27 |
| ATOM | 3512 | N | PRO | 663 | 49.448 | 12.549 | 13.895 | 1.00 | 36.46 |
| ATOM | 3513 | CD | PRO | 663 | 50.320 | 13.216 | 12.914 | 1.00 | 38.35 |
| ATOM | 3514 | CA | PRO | 663 | 50.224 | 12.148 | 15.070 | 1.00 | 35.98 |
| ATOM | 3515 | CB | PRO | 663 | 51.537 | 12.887 | 14.872 | 1.00 | 34.95 |
| ATOM | 3516 | CG | PRO | 663 | 51.702 | 12.836 | 13.403 | 1.00 | 39.18 |
| ATOM | 3517 | C | PRO | 663 | 49.569 | 12.499 | 16.398 | 1.00 | 35.53 |
| ATOM | 3518 | O | PRO | 663 | 49.779 | 11.814 | 17.399 | 1.00 | 38.34 |
| ATOM | 3519 | N | VAL | 664 | 48.759 | 13.558 | 16.414 | 1.00 | 32.71 |
| ATOM | 3520 | CA | VAL | 664 | 48.080 | 13.964 | 17.632 | 1.00 | 30.18 |
| ATOM | 3521 | CB | VAL | 664 | 47.195 | 15.242 | 17.427 | 1.00 | 31.31 |
| ATOM | 3522 | CG1 | VAL | 664 | 48.060 | 16.409 | 17.038 | 1.00 | 28.93 |
| ATOM | 3523 | CG2 | VAL | 664 | 46.143 | 15.038 | 16.345 | 1.00 | 34.42 |
| ATOM | 3524 | C | VAL | 664 | 47.268 | 12.787 | 18.172 | 1.00 | 29.48 |
| ATOM | 3525 | O | VAL | 664 | 47.080 | 12.654 | 19.388 | 1.00 | 30.41 |
| ATOM | 3526 | N | LYS | 665 | 46.873 | 11.883 | 17.282 | 1.00 | 29.29 |
| ATOM | 3527 | CA | LYS | 665 | 46.105 | 10.704 | 17.668 | 1.00 | 28.55 |
| ATOM | 3528 | CB | LYS | 665 | 45.517 | 10.037 | 16.423 | 1.00 | 26.97 |
| ATOM | 3529 | CG | LYS | 665 | 44.415 | 10.873 | 15.786 | 1.00 | 27.88 |
| ATOM | 3530 | CD | LYS | 665 | 43.979 | 10.366 | 14.418 | 1.00 | 29.41 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3531 | CE | LYS | 665 | 42.785 | 11.162 | 13.899 | 1.00 | 26.35 |
| ATOM | 3532 | NZ | LYS | 665 | 42.363 | 10.809 | 12.508 | 1.00 | 26.16 |
| ATOM | 3533 | C | LYS | 665 | 46.890 | 9.730 | 18.556 | 1.00 | 28.81 |
| ATOM | 3534 | O | LYS | 665 | 46.315 | 8.802 | 19.113 | 1.00 | 29.38 |
| ATOM | 3535 | N | TRP | 666 | 48.181 | 9.976 | 18.736 | 1.00 | 28.98 |
| ATOM | 3536 | CA | TRP | 666 | 49.005 | 9.128 | 19.599 | 1.00 | 31.67 |
| ATOM | 3537 | CB | TRP | 666 | 50.323 | 8.755 | 18.913 | 1.00 | 29.46 |
| ATOM | 3538 | CG | TRP | 666 | 50.205 | 7.582 | 17.977 | 1.00 | 28.92 |
| ATOM | 3539 | CD2 | TRP | 666 | 49.676 | 7.603 | 16.642 | 1.00 | 27.62 |
| ATOM | 3540 | CE2 | TRP | 666 | 49.740 | 6.276 | 16.162 | 1.00 | 27.15 |
| ATOM | 3541 | CE3 | TRP | 666 | 49.151 | 8.607 | 15.818 | 1.00 | 25.27 |
| ATOM | 3542 | CD1 | TRP | 666 | 50.565 | 6.289 | 18.238 | 1.00 | 24.30 |
| ATOM | 3543 | NE1 | TRP | 666 | 50.287 | 5.506 | 17.147 | 1.00 | 27.82 |
| ATOM | 3544 | CZ2 | TRP | 666 | 49.295 | 5.930 | 14.872 | 1.00 | 26.95 |
| ATOM | 3545 | CZ3 | TRP | 666 | 48.707 | 8.256 | 14.536 | 1.00 | 25.95 |
| ATOM | 3546 | CH2 | TRP | 666 | 48.778 | 6.929 | 14.081 | 1.00 | 28.35 |
| ATOM | 3547 | C | TRP | 666 | 49.316 | 9.836 | 20.907 | 1.00 | 33.46 |
| ATOM | 3548 | O | TRP | 666 | 49.790 | 9.219 | 21.867 | 1.00 | 34.77 |
| ATOM | 3549 | N | MET | 667 | 49.021 | 11.128 | 20.947 | 1.00 | 35.61 |
| ATOM | 3550 | CA | MET | 667 | 49.306 | 11.948 | 22.110 | 1.00 | 37.94 |
| ATOM | 3551 | CB | MET | 667 | 49.308 | 13.419 | 21.723 | 1.00 | 40.22 |
| ATOM | 3552 | CG | MET | 667 | 50.606 | 13.939 | 21.150 | 1.00 | 40.77 |
| ATOM | 3553 | SD | MET | 667 | 50.479 | 15.723 | 20.906 | 1.00 | 44.04 |
| ATOM | 3554 | CE | MET | 667 | 50.932 | 15.858 | 19.204 | 1.00 | 39.07 |
| ATOM | 3555 | C | MET | 667 | 48.432 | 11.775 | 23.346 | 1.00 | 39.61 |
| ATOM | 3556 | O | MET | 667 | 47.211 | 11.672 | 23.255 | 1.00 | 42.46 |
| ATOM | 3557 | N | ALA | 668 | 49.072 | 11.820 | 24.505 | 1.00 | 38.46 |
| ATOM | 3558 | CA | ALA | 668 | 48.383 | 11.704 | 25.773 | 1.00 | 37.78 |
| ATOM | 3559 | CB | ALA | 668 | 49.388 | 11.473 | 26.894 | 1.00 | 38.21 |
| ATOM | 3560 | C | ALA | 668 | 47.666 | 13.033 | 25.966 | 1.00 | 37.46 |
| ATOM | 3561 | O | ALA | 668 | 48.156 | 14.072 | 25.521 | 1.00 | 35.74 |
| ATOM | 3562 | N | PRO | 669 | 46.521 | 13.027 | 26.665 | 1.00 | 37.55 |
| ATOM | 3563 | CD | PRO | 669 | 45.868 | 11.840 | 27.243 | 1.00 | 38.19 |
| ATOM | 3564 | CA | PRO | 669 | 45.723 | 14.229 | 26.923 | 1.00 | 39.30 |
| ATOM | 3565 | CB | PRO | 669 | 44.638 | 13.708 | 27.864 | 1.00 | 39.82 |
| ATOM | 3566 | CG | PRO | 669 | 44.444 | 12.301 | 27.379 | 1.00 | 39.13 |
| ATOM | 3567 | C | PRO | 669 | 46.517 | 15.391 | 27.535 | 1.00 | 40.55 |
| ATOM | 3568 | O | PRO | 669 | 46.442 | 16.523 | 27.056 | 1.00 | 39.87 |
| ATOM | 3569 | N | GLU | 670 | 47.303 | 15.113 | 28.569 | 1.00 | 41.15 |
| ATOM | 3570 | CA | GLU | 670 | 48.096 | 16.169 | 29.200 | 1.00 | 42.80 |
| ATOM | 3571 | CB | GLU | 670 | 48.776 | 15.657 | 30.464 | 1.00 | 42.97 |
| ATOM | 3572 | CG | GLU | 670 | 49.928 | 14.705 | 30.205 | 1.00 | 42.82 |
| ATOM | 3573 | CD | GLU | 670 | 49.506 | 13.252 | 30.150 | 1.00 | 44.16 |
| ATOM | 3574 | OE1 | GLU | 670 | 50.395 | 12.384 | 30.257 | 1.00 | 40.43 |
| ATOM | 3575 | OE2 | GLU | 670 | 48.297 | 12.974 | 30.013 | 1.00 | 46.36 |
| ATOM | 3576 | C | GLU | 670 | 49.145 | 16.795 | 28.276 | 1.00 | 43.00 |
| ATOM | 3577 | O | GLU | 670 | 49.435 | 17.979 | 28.380 | 1.00 | 40.37 |
| ATOM | 3578 | N | ALA | 671 | 49.697 | 15.999 | 27.367 | 1.00 | 44.03 |
| ATOM | 3579 | CA | ALA | 671 | 50.708 | 16.495 | 26.440 | 1.00 | 44.90 |
| ATOM | 3580 | CB | ALA | 671 | 51.460 | 15.333 | 25.814 | 1.00 | 42.47 |
| ATOM | 3581 | C | ALA | 671 | 50.063 | 17.364 | 25.361 | 1.00 | 47.79 |
| ATOM | 3582 | O | ALA | 671 | 50.602 | 18.398 | 24.977 | 1.00 | 47.27 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3583 | N | LEU | 672 | 48.877 | 16.952 | 24.922 | 1.00 | 51.20 |
| ATOM | 3584 | CA | LEU | 672 | 48.131 | 17.650 | 23.881 | 1.00 | 52.90 |
| ATOM | 3585 | CB | LEU | 672 | 47.092 | 16.685 | 23.288 | 1.00 | 54.84 |
| ATOM | 3586 | CG | LEU | 672 | 46.307 | 17.010 | 22.015 | 1.00 | 57.19 |
| ATOM | 3587 | CD1 | LEU | 672 | 47.230 | 17.328 | 20.869 | 1.00 | 57.53 |
| ATOM | 3588 | CD2 | LEU | 672 | 45.443 | 15.813 | 21.659 | 1.00 | 56.95 |
| ATOM | 3589 | C | LEU | 672 | 47.456 | 18.913 | 24.445 | 1.00 | 53.45 |
| ATOM | 3590 | O | LEU | 672 | 47.502 | 19.988 | 23.841 | 1.00 | 52.71 |
| ATOM | 3591 | N | PHE | 673 | 46.866 | 18.777 | 25.627 | 1.00 | 53.82 |
| ATOM | 3592 | CA | PHE | 673 | 46.179 | 19.878 | 26.281 | 1.00 | 55.95 |
| ATOM | 3593 | CB | PHE | 673 | 44.974 | 19.340 | 27.060 | 1.00 | 53.37 |
| ATOM | 3594 | CG | PHE | 673 | 43.967 | 18.612 | 26.200 | 1.00 | 52.79 |
| ATOM | 3595 | CD1 | PHE | 673 | 43.477 | 17.368 | 26.580 | 1.00 | 54.64 |
| ATOM | 3596 | CD2 | PHE | 673 | 43.491 | 19.173 | 25.022 | 1.00 | 53.89 |
| ATOM | 3597 | CE1 | PHE | 673 | 42.530 | 16.702 | 25.808 | 1.00 | 55.44 |
| ATOM | 3598 | CE2 | PHE | 673 | 42.540 | 18.507 | 24.239 | 1.00 | 54.80 |
| ATOM | 3599 | CZ | PHE | 673 | 42.062 | 17.269 | 24.637 | 1.00 | 54.86 |
| ATOM | 3600 | C | PHE | 673 | 47.071 | 20.733 | 27.200 | 1.00 | 58.97 |
| ATOM | 3601 | O | PHE | 673 | 47.084 | 21.959 | 27.095 | 1.00 | 60.79 |
| ATOM | 3602 | N | ASP | 674 | 47.832 | 20.086 | 28.077 | 1.00 | 60.63 |
| ATOM | 3603 | CA | ASP | 674 | 48.698 | 20.798 | 29.026 | 1.00 | 61.52 |
| ATOM | 3604 | CB | ASP | 674 | 48.638 | 20.137 | 30.410 | 1.00 | 61.39 |
| ATOM | 3605 | CG | ASP | 674 | 47.247 | 20.143 | 31.010 | 1.00 | 62.87 |
| ATOM | 3606 | OD1 | ASP | 674 | 46.706 | 19.039 | 31.246 | 1.00 | 62.99 |
| ATOM | 3607 | OD2 | ASP | 674 | 46.698 | 21.239 | 31.253 | 1.00 | 63.55 |
| ATOM | 3608 | C | ASP | 674 | 50.176 | 20.898 | 28.618 | 1.00 | 61.58 |
| ATOM | 3609 | O | ASP | 674 | 51.014 | 21.284 | 29.446 | 1.00 | 60.41 |
| ATOM | 3610 | N | ARG | 675 | 50.499 | 20.519 | 27.380 | 1.00 | 61.38 |
| ATOM | 3611 | CA | ARG | 675 | 51.885 | 20.526 | 26.883 | 1.00 | 59.23 |
| ATOM | 3612 | CB | ARG | 675 | 52.336 | 21.944 | 26.515 | 1.00 | 59.05 |
| ATOM | 3613 | CG | ARG | 675 | 51.548 | 22.564 | 25.367 | 1.00 | 64.48 |
| ATOM | 3614 | CD | ARG | 675 | 52.036 | 23.967 | 25.014 | 1.00 | 68.61 |
| ATOM | 3615 | NE | ARG | 675 | 53.348 | 23.969 | 24.359 | 1.00 | 69.16 |
| ATOM | 3616 | CZ | ARG | 675 | 54.076 | 25.061 | 24.145 | 1.00 | 68.19 |
| ATOM | 3617 | NH1 | ARG | 675 | 53.622 | 26.250 | 24.531 | 1.00 | 66.97 |
| ATOM | 3618 | NH2 | ARG | 675 | 55.265 | 24.965 | 23.564 | 1.00 | 67.00 |
| ATOM | 3619 | C | ARG | 675 | 52.849 | 19.885 | 27.892 | 1.00 | 57.27 |
| ATOM | 3620 | O | ARG | 675 | 54.002 | 20.300 | 28.033 | 1.00 | 57.05 |
| ATOM | 3621 | N | ILE | 676 | 52.356 | 18.867 | 28.591 | 1.00 | 55.44 |
| ATOM | 3622 | CA | ILE | 676 | 53.136 | 18.140 | 29.589 | 1.00 | 53.31 |
| ATOM | 3623 | CB | ILE | 676 | 52.314 | 17.899 | 30.874 | 1.00 | 50.96 |
| ATOM | 3624 | CG2 | ILE | 676 | 52.934 | 16.787 | 31.718 | 1.00 | 47.57 |
| ATOM | 3625 | CG1 | ILE | 676 | 52.213 | 19.196 | 31.669 | 1.00 | 50.88 |
| ATOM | 3626 | CD1 | ILE | 676 | 51.443 | 19.073 | 32.964 | 1.00 | 53.09 |
| ATOM | 3627 | C | ILE | 676 | 53.608 | 16.801 | 29.029 | 1.00 | 54.75 |
| ATOM | 3628 | O | ILE | 676 | 52.810 | 15.891 | 28.824 | 1.00 | 57.06 |
| ATOM | 3629 | N | TYR | 677 | 54.902 | 16.681 | 28.777 | 1.00 | 53.61 |
| ATOM | 3630 | CA | TYR | 677 | 55.459 | 15.447 | 28.243 | 1.00 | 52.80 |
| ATOM | 3631 | CB | TYR | 677 | 56.332 | 15.747 | 27.023 | 1.00 | 53.40 |
| ATOM | 3632 | CG | TYR | 677 | 55.554 | 16.184 | 25.794 | 1.00 | 57.32 |
| ATOM | 3633 | CD1 | TYR | 677 | 55.256 | 17.535 | 25.575 | 1.00 | 55.94 |
| ATOM | 3634 | CE1 | TYR | 677 | 54.574 | 17.946 | 24.436 | 1.00 | 54.18 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3635 | CD2 | TYR | 677 | 55.140 | 15.251 | 24.829 | 1.00 | 56.63 |
| ATOM | 3636 | CE2 | TYR | 677 | 54.459 | 15.654 | 23.680 | 1.00 | 54.84 |
| ATOM | 3637 | CZ | TYR | 677 | 54.183 | 17.004 | 23.490 | 1.00 | 56.38 |
| ATOM | 3638 | OH | TYR | 677 | 53.555 | 17.426 | 22.340 | 1.00 | 57.46 |
| ATOM | 3639 | C | TYR | 677 | 56.268 | 14.713 | 29.304 | 1.00 | 51.49 |
| ATOM | 3640 | O | TYR | 677 | 57.186 | 15.283 | 29.904 | 1.00 | 52.65 |
| ATOM | 3641 | N | THR | 678 | 55.881 | 13.471 | 29.579 | 1.00 | 48.54 |
| ATOM | 3642 | CA | THR | 678 | 56.571 | 12.648 | 30.568 | 1.00 | 46.14 |
| ATOM | 3643 | CB | THR | 678 | 55.776 | 12.597 | 31.910 | 1.00 | 47.34 |
| ATOM | 3644 | OG1 | THR | 678 | 54.615 | 11.764 | 31.764 | 1.00 | 50.96 |
| ATOM | 3645 | CG2 | THR | 678 | 55.346 | 13.996 | 32.345 | 1.00 | 47.47 |
| ATOM | 3646 | C | THR | 678 | 56.742 | 11.218 | 30.041 | 1.00 | 43.21 |
| ATOM | 3647 | O | THR | 678 | 56.371 | 10.917 | 28.912 | 1.00 | 41.64 |
| ATOM | 3648 | N | HIS | 679 | 57.334 | 10.351 | 30.854 | 1.00 | 42.21 |
| ATOM | 3649 | CA | HIS | 679 | 57.507 | 8.969 | 30.456 | 1.00 | 39.96 |
| ATOM | 3650 | CB | HIS | 679 | 58.410 | 8.216 | 31.428 | 1.00 | 39.23 |
| ATOM | 3651 | CG | HIS | 679 | 59.833 | 8.677 | 31.418 | 1.00 | 43.24 |
| ATOM | 3652 | CD2 | HIS | 679 | 60.501 | 9.505 | 32.253 | 1.00 | 43.12 |
| ATOM | 3653 | ND1 | HIS | 679 | 60.759 | 8.236 | 30.498 | 1.00 | 42.63 |
| ATOM | 3654 | CE1 | HIS | 679 | 61.938 | 8.762 | 30.774 | 1.00 | 42.66 |
| ATOM | 3655 | NE2 | HIS | 679 | 61.807 | 9.539 | 31.832 | 1.00 | 43.80 |
| ATOM | 3656 | C | HIS | 679 | 56.145 | 8.301 | 30.429 | 1.00 | 40.78 |
| ATOM | 3657 | O | HIS | 679 | 55.930 | 7.358 | 29.678 | 1.00 | 42.66 |
| ATOM | 3658 | N | GLN | 680 | 55.227 | 8.803 | 31.254 | 1.00 | 40.26 |
| ATOM | 3659 | CA | GLN | 680 | 53.881 | 8.261 | 31.324 | 1.00 | 39.10 |
| ATOM | 3660 | CB | GLN | 680 | 53.187 | 8.664 | 32.625 | 1.00 | 39.23 |
| ATOM | 3661 | CG | GLN | 680 | 53.762 | 7.980 | 33.874 | 1.00 | 41.07 |
| ATOM | 3662 | CD | GLN | 680 | 53.813 | 6.450 | 33.770 | 1.00 | 39.96 |
| ATOM | 3663 | OE1 | GLN | 680 | 52.818 | 5.762 | 33.993 | 1.00 | 39.53 |
| ATOM | 3664 | NE2 | GLN | 680 | 54.990 | 5.919 | 33.464 | 1.00 | 32.85 |
| ATOM | 3665 | C | GLN | 680 | 53.070 | 8.676 | 30.103 | 1.00 | 39.20 |
| ATOM | 3666 | O | GLN | 680 | 52.194 | 7.933 | 29.656 | 1.00 | 39.29 |
| ATOM | 3667 | N | SER | 681 | 53.368 | 9.843 | 29.531 | 1.00 | 38.01 |
| ATOM | 3668 | CA | SER | 681 | 52.656 | 10.264 | 28.325 | 1.00 | 39.27 |
| ATOM | 3669 | CB | SER | 681 | 52.979 | 11.712 | 27.968 | 1.00 | 40.93 |
| ATOM | 3670 | OG | SER | 681 | 54.366 | 11.936 | 27.943 | 1.00 | 39.70 |
| ATOM | 3671 | C | SER | 681 | 53.090 | 9.309 | 27.208 | 1.00 | 39.93 |
| ATOM | 3672 | O | SER | 681 | 52.285 | 8.953 | 26.335 | 1.00 | 40.46 |
| ATOM | 3673 | N | ASP | 682 | 54.356 | 8.881 | 27.269 | 1.00 | 37.28 |
| ATOM | 3674 | CA | ASP | 682 | 54.920 | 7.921 | 26.315 | 1.00 | 35.38 |
| ATOM | 3675 | CB | ASP | 682 | 56.411 | 7.673 | 26.586 | 1.00 | 33.58 |
| ATOM | 3676 | CG | ASP | 682 | 57.332 | 8.520 | 25.717 | 1.00 | 33.16 |
| ATOM | 3677 | OD1 | ASP | 682 | 58.545 | 8.283 | 25.828 | 1.00 | 31.76 |
| ATOM | 3678 | OD2 | ASP | 682 | 56.886 | 9.391 | 24.936 | 1.00 | 30.06 |
| ATOM | 3679 | C | ASP | 682 | 54.178 | 6.599 | 26.463 | 1.00 | 34.70 |
| ATOM | 3680 | O | ASP | 682 | 54.012 | 5.868 | 25.488 | 1.00 | 35.67 |
| ATOM | 3681 | N | VAL | 683 | 53.758 | 6.296 | 27.691 | 1.00 | 34.44 |
| ATOM | 3682 | CA | VAL | 683 | 53.011 | 5.072 | 27.987 | 1.00 | 35.14 |
| ATOM | 3683 | CB | VAL | 683 | 52.895 | 4.852 | 29.544 | 1.00 | 35.48 |
| ATOM | 3684 | CG1 | VAL | 683 | 51.752 | 3.900 | 29.890 | 1.00 | 34.95 |
| ATOM | 3685 | CG2 | VAL | 683 | 54.202 | 4.282 | 30.080 | 1.00 | 28.77 |
| ATOM | 3686 | C | VAL | 683 | 51.638 | 5.091 | 27.279 | 1.00 | 32.81 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3687 | O | VAL | 683 | 51.173 | 4.050 | 26.801 | 1.00 | 31.24 |
| ATOM | 3688 | N | TRP | 684 | 51.018 | 6.271 | 27.187 | 1.00 | 30.88 |
| ATOM | 3689 | CA | TRP | 684 | 49.731 | 6.426 | 26.502 | 1.00 | 31.79 |
| ATOM | 3690 | CB | TRP | 684 | 49.189 | 7.849 | 26.679 | 1.00 | 34.88 |
| ATOM | 3691 | CG | TRP | 684 | 47.972 | 8.173 | 25.833 | 1.00 | 37.61 |
| ATOM | 3692 | CD2 | TRP | 684 | 46.635 | 8.396 | 26.305 | 1.00 | 39.13 |
| ATOM | 3693 | CE2 | TRP | 684 | 45.851 | 8.741 | 25.184 | 1.00 | 38.42 |
| ATOM | 3694 | CE3 | TRP | 684 | 46.024 | 8.349 | 27.567 | 1.00 | 39.05 |
| ATOM | 3695 | CD1 | TRP | 684 | 47.938 | 8.374 | 24.476 | 1.00 | 36.48 |
| ATOM | 3696 | NE1 | TRP | 684 | 46.669 | 8.720 | 24.085 | 1.00 | 38.70 |
| ATOM | 3697 | CZ2 | TRP | 684 | 44.483 | 9.036 | 25.290 | 1.00 | 37.82 |
| ATOM | 3698 | CZ3 | TRP | 684 | 44.668 | 8.644 | 27.664 | 1.00 | 38.19 |
| ATOM | 3699 | CH2 | TRP | 684 | 43.918 | 8.980 | 26.536 | 1.00 | 37.68 |
| ATOM | 3700 | C | TRP | 684 | 49.947 | 6.131 | 25.020 | 1.00 | 31.09 |
| ATOM | 3701 | O | TRP | 684 | 49.214 | 5.332 | 24.430 | 1.00 | 32.25 |
| ATOM | 3702 | N | SER | 685 | 50.977 | 6.750 | 24.444 | 1.00 | 28.90 |
| ATOM | 3703 | CA | SER | 685 | 51.345 | 6.536 | 23.052 | 1.00 | 27.10 |
| ATOM | 3704 | CB | SER | 685 | 52.620 | 7.312 | 22.748 | 1.00 | 23.88 |
| ATOM | 3705 | OG | SER | 685 | 52.459 | 8.710 | 22.974 | 1.00 | 25.82 |
| ATOM | 3706 | C | SER | 685 | 51.567 | 5.028 | 22.786 | 1.00 | 27.85 |
| ATOM | 3707 | O | SER | 685 | 51.172 | 4.493 | 21.746 | 1.00 | 28.89 |
| ATOM | 3708 | N | PHE | 686 | 52.178 | 4.334 | 23.741 | 1.00 | 28.84 |
| ATOM | 3709 | CA | PHE | 686 | 52.410 | 2.893 | 23.622 | 1.00 | 27.86 |
| ATOM | 3710 | CB | PHE | 686 | 53.255 | 2.403 | 24.800 | 1.00 | 28.14 |
| ATOM | 3711 | CG | PHE | 686 | 53.498 | 0.914 | 24.803 | 1.00 | 28.41 |
| ATOM | 3712 | CD1 | PHE | 686 | 54.256 | 0.313 | 23.802 | 1.00 | 27.54 |
| ATOM | 3713 | CD2 | PHE | 686 | 52.949 | 0.109 | 25.796 | 1.00 | 29.15 |
| ATOM | 3714 | CE1 | PHE | 686 | 54.465 | -1.057 | 23.792 | 1.00 | 24.25 |
| ATOM | 3715 | CE2 | PHE | 686 | 53.151 | -1.268 | 25.790 | 1.00 | 27.86 |
| ATOM | 3716 | CZ | PHE | 686 | 53.912 | -1.850 | 24.782 | 1.00 | 26.09 |
| ATOM | 3717 | C | PHE | 686 | 51.072 | 2.122 | 23.566 | 1.00 | 30.99 |
| ATOM | 3718 | O | PHE | 686 | 50.960 | 1.109 | 22.873 | 1.00 | 29.21 |
| ATOM | 3719 | N | GLY | 687 | 50.051 | 2.603 | 24.286 | 1.00 | 30.57 |
| ATOM | 3720 | CA | GLY | 687 | 48.758 | 1.939 | 24.273 | 1.00 | 31.78 |
| ATOM | 3721 | C | GLY | 687 | 48.202 | 1.923 | 22.862 | 1.00 | 32.51 |
| ATOM | 3722 | O | GLY | 687 | 47.687 | 0.908 | 22.373 | 1.00 | 31.25 |
| ATOM | 3723 | N | VAL | 688 | 48.292 | 3.073 | 22.204 | 1.00 | 32.58 |
| ATOM | 3724 | CA | VAL | 688 | 47.825 | 3.202 | 20.827 | 1.00 | 30.66 |
| ATOM | 3725 | CB | VAL | 688 | 47.804 | 4.684 | 20.362 | 1.00 | 28.55 |
| ATOM | 3726 | CG1 | VAL | 688 | 47.231 | 4.795 | 18.950 | 1.00 | 27.25 |
| ATOM | 3727 | CG2 | VAL | 688 | 46.944 | 5.522 | 21.320 | 1.00 | 27.12 |
| ATOM | 3728 | C | VAL | 688 | 48.684 | 2.326 | 19.910 | 1.00 | 29.96 |
| ATOM | 3729 | O | VAL | 688 | 48.160 | 1.731 | 18.974 | 1.00 | 30.83 |
| ATOM | 3730 | N | LEU | 689 | 49.973 | 2.202 | 20.219 | 1.00 | 30.02 |
| ATOM | 3731 | CA | LEU | 689 | 50.893 | 1.371 | 19.430 | 1.00 | 30.48 |
| ATOM | 3732 | CB | LEU | 689 | 52.359 | 1.571 | 19.877 | 1.00 | 28.13 |
| ATOM | 3733 | CG | LEU | 689 | 53.466 | 0.966 | 18.995 | 1.00 | 26.34 |
| ATOM | 3734 | CD1 | LEU | 689 | 54.790 | 1.697 | 19.174 | 1.00 | 25.54 |
| ATOM | 3735 | CD2 | LEU | 689 | 53.628 | -0.505 | 19.264 | 1.00 | 24.99 |
| ATOM | 3736 | C | LEU | 689 | 50.479 | -0.096 | 19.567 | 1.00 | 30.54 |
| ATOM | 3737 | O | LEU | 689 | 50.540 | -0.849 | 18.602 | 1.00 | 27.86 |
| ATOM | 3738 | N | LEU | 690 | 50.013 | -0.468 | 20.759 | 1.00 | 33.73 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3739 | CA | LEU | 690 | 49.553 | -1.830 | 21.029 | 1.00 | 32.47 |
| ATOM | 3740 | CB | LEU | 690 | 49.141 | -1.982 | 22.496 | 1.00 | 31.82 |
| ATOM | 3741 | CG | LEU | 690 | 50.136 | -2.220 | 23.634 | 1.00 | 29.71 |
| ATOM | 3742 | CD1 | LEU | 690 | 49.396 | -2.129 | 24.956 | 1.00 | 31.53 |
| ATOM | 3743 | CD2 | LEU | 690 | 50.771 | -3.605 | 23.483 | 1.00 | 31.69 |
| ATOM | 3744 | C | LEU | 690 | 48.335 | -2.101 | 20.136 | 1.00 | 33.01 |
| ATOM | 3745 | O | LEU | 690 | 48.223 | -3.168 | 19.521 | 1.00 | 32.68 |
| ATOM | 3746 | N | TRP | 691 | 47.423 | -1.131 | 20.089 | 1.00 | 32.37 |
| ATOM | 3747 | CA | TRP | 691 | 46.230 | -1.215 | 19.256 | 1.00 | 32.11 |
| ATOM | 3748 | CB | TRP | 691 | 45.424 | 0.083 | 19.373 | 1.00 | 33.19 |
| ATOM | 3749 | CG | TRP | 691 | 44.086 | 0.055 | 18.678 | 1.00 | 33.95 |
| ATOM | 3750 | CD2 | TRP | 691 | 43.812 | 0.469 | 17.337 | 1.00 | 30.48 |
| ATOM | 3751 | CE2 | TRP | 691 | 42.434 | 0.294 | 17.118 | 1.00 | 32.75 |
| ATOM | 3752 | CE3 | TRP | 691 | 44.599 | 0.989 | 16.301 | 1.00 | 29.47 |
| ATOM | 3753 | CD1 | TRP | 691 | 42.889 | -0.352 | 19.199 | 1.00 | 34.34 |
| ATOM | 3754 | NE1 | TRP | 691 | 41.894 | -0.211 | 18.272 | 1.00 | 36.53 |
| ATOM | 3755 | CZ2 | TRP | 691 | 41.831 | 0.601 | 15.900 | 1.00 | 30.85 |
| ATOM | 3756 | CZ3 | TRP | 691 | 44.003 | 1.289 | 15.100 | 1.00 | 30.51 |
| ATOM | 3757 | CH2 | TRP | 691 | 42.630 | 1.104 | 14.907 | 1.00 | 30.29 |
| ATOM | 3758 | C | TRP | 691 | 46.661 | -1.421 | 17.805 | 1.00 | 31.49 |
| ATOM | 3759 | O | TRP | 691 | 46.062 | -2.221 | 17.092 | 1.00 | 31.20 |
| ATOM | 3760 | N | GLU | 692 | 47.669 | -0.656 | 17.374 | 1.00 | 32.90 |
| ATOM | 3761 | CA | GLU | 692 | 48.207 | -0.734 | 16.019 | 1.00 | 29.78 |
| ATOM | 3762 | CB | GLU | 692 | 49.383 | 0.233 | 15.809 | 1.00 | 25.56 |
| ATOM | 3763 | CG | GLU | 692 | 49.009 | 1.696 | 15.713 | 1.00 | 25.85 |
| ATOM | 3764 | CD | GLU | 692 | 50.195 | 2.570 | 15.363 | 1.00 | 27.76 |
| ATOM | 3765 | OE1 | GLU | 692 | 51.001 | 2.850 | 16.265 | 1.00 | 29.52 |
| ATOM | 3766 | OE2 | GLU | 692 | 50.333 | 2.981 | 14.191 | 1.00 | 26.84 |
| ATOM | 3767 | C | GLU | 692 | 48.682 | -2.136 | 15.696 | 1.00 | 31.08 |
| ATOM | 3768 | O | GLU | 692 | 48.545 | -2.593 | 14.553 | 1.00 | 32.57 |
| ATOM | 3769 | N | ILE | 693 | 49.262 | -2.804 | 16.689 | 1.00 | 31.81 |
| ATOM | 3770 | CA | ILE | 693 | 49.774 | -4.163 | 16.506 | 1.00 | 31.87 |
| ATOM | 3771 | CB | ILE | 693 | 50.666 | -4.614 | 17.699 | 1.00 | 33.50 |
| ATOM | 3772 | CG2 | ILE | 693 | 51.140 | -6.075 | 17.513 | 1.00 | 33.06 |
| ATOM | 3773 | CG1 | ILE | 693 | 51.879 | -3.703 | 17.827 | 1.00 | 34.04 |
| ATOM | 3774 | CD1 | ILE | 693 | 52.744 | -4.008 | 19.025 | 1.00 | 31.52 |
| ATOM | 3775 | C | ILE | 693 | 48.643 | -5.177 | 16.335 | 1.00 | 31.43 |
| ATOM | 3776 | O | ILE | 693 | 48.633 | -5.982 | 15.403 | 1.00 | 29.55 |
| ATOM | 3777 | N | PHE | 694 | 47.654 | -5.087 | 17.207 | 1.00 | 33.58 |
| ATOM | 3778 | CA | PHE | 694 | 46.550 | -6.027 | 17.178 | 1.00 | 36.72 |
| ATOM | 3779 | CB | PHE | 694 | 45.980 | -6.179 | 18.589 | 1.00 | 36.27 |
| ATOM | 3780 | CG | PHE | 694 | 46.988 | -6.724 | 19.547 | 1.00 | 34.29 |
| ATOM | 3781 | CD1 | PHE | 694 | 47.500 | -5.949 | 20.581 | 1.00 | 34.95 |
| ATOM | 3782 | CD2 | PHE | 694 | 47.560 | -7.972 | 19.297 | 1.00 | 31.60 |
| ATOM | 3783 | CE1 | PHE | 694 | 48.576 | -6.413 | 21.344 | 1.00 | 35.73 |
| ATOM | 3784 | CE2 | PHE | 694 | 48.633 | -8.443 | 20.049 | 1.00 | 31.12 |
| ATOM | 3785 | CZ | PHE | 694 | 49.149 | -7.661 | 21.066 | 1.00 | 33.97 |
| ATOM | 3786 | C | PHE | 694 | 45.516 | -5.870 | 16.065 | 1.00 | 37.70 |
| ATOM | 3787 | O | PHE | 694 | 44.684 | -6.756 | 15.839 | 1.00 | 37.99 |
| ATOM | 3788 | N | THR | 695 | 45.604 | -4.745 | 15.355 | 1.00 | 36.11 |
| ATOM | 3789 | CA | THR | 695 | 44.747 | -4.485 | 14.205 | 1.00 | 31.23 |
| ATOM | 3790 | CB | THR | 695 | 44.107 | -3.081 | 14.236 | 1.00 | 30.49 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3791 | OG1 | THR | 695 | 45.133 | -2.079 | 14.134 | 1.00 | 30.14 |
| ATOM | 3792 | CG2 | THR | 695 | 43.329 | -2.888 | 15.512 | 1.00 | 31.07 |
| ATOM | 3793 | C | THR | 695 | 45.612 | -4.619 | 12.965 | 1.00 | 29.79 |
| ATOM | 3794 | O | THR | 695 | 45.163 | -4.325 | 11.862 | 1.00 | 31.31 |
| ATOM | 3795 | N | LEU | 696 | 46.859 | -5.051 | 13.164 | 1.00 | 29.75 |
| ATOM | 3796 | CA | LEU | 696 | 47.826 | -5.259 | 12.081 | 1.00 | 28.46 |
| ATOM | 3797 | CB | LEU | 696 | 47.456 | -6.495 | 11.245 | 1.00 | 29.96 |
| ATOM | 3798 | CG | LEU | 696 | 47.281 | -7.848 | 11.946 | 1.00 | 30.38 |
| ATOM | 3799 | CD1 | LEU | 696 | 47.142 | -8.941 | 10.909 | 1.00 | 30.43 |
| ATOM | 3800 | CD2 | LEU | 696 | 48.468 | -8.138 | 12.800 | 1.00 | 32.35 |
| ATOM | 3801 | C | LEU | 696 | 48.101 | -4.076 | 11.160 | 1.00 | 28.76 |
| ATOM | 3802 | O | LEU | 696 | 48.210 | -4.235 | 9.946 | 1.00 | 26.97 |
| ATOM | 3803 | N | GLY | 697 | 48.314 | -2.900 | 11.745 | 1.00 | 32.70 |
| ATOM | 3804 | CA | GLY | 697 | 48.608 | -1.705 | 10.960 | 1.00 | 31.69 |
| ATOM | 3805 | C | GLY | 697 | 47.432 | -0.763 | 10.817 | 1.00 | 32.24 |
| ATOM | 3806 | O | GLY | 697 | 47.398 | 0.099 | 9.941 | 1.00 | 31.81 |
| ATOM | 3807 | N | GLY | 698 | 46.455 | -0.922 | 11.700 | 1.00 | 32.63 |
| ATOM | 3808 | CA | GLY | 698 | 45.277 | -0.081 | 11.643 | 1.00 | 31.93 |
| ATOM | 3809 | C | GLY | 698 | 45.504 | 1.411 | 11.820 | 1.00 | 28.95 |
| ATOM | 3810 | O | GLY | 698 | 46.454 | 1.858 | 12.449 | 1.00 | 26.05 |
| ATOM | 3811 | N | SER | 699 | 44.569 | 2.174 | 11.282 | 1.00 | 30.03 |
| ATOM | 3812 | CA | SER | 699 | 44.608 | 3.618 | 11.352 | 1.00 | 30.52 |
| ATOM | 3813 | CB | SER | 699 | 44.095 | 4.219 | 10.046 | 1.00 | 31.24 |
| ATOM | 3814 | OG | SER | 699 | 44.047 | 5.639 | 10.095 | 1.00 | 33.61 |
| ATOM | 3815 | C | SER | 699 | 43.695 | 4.024 | 12.492 | 1.00 | 30.45 |
| ATOM | 3816 | O | SER | 699 | 42.490 | 3.755 | 12.450 | 1.00 | 29.11 |
| ATOM | 3817 | N | PRO | 700 | 44.259 | 4.591 | 13.573 | 1.00 | 32.27 |
| ATOM | 3818 | CD | PRO | 700 | 45.693 | 4.761 | 13.881 | 1.00 | 29.61 |
| ATOM | 3819 | CA | PRO | 700 | 43.408 | 5.007 | 14.695 | 1.00 | 31.34 |
| ATOM | 3820 | CB | PRO | 700 | 44.428 | 5.358 | 15.777 | 1.00 | 31.30 |
| ATOM | 3821 | CG | PRO | 700 | 45.662 | 5.745 | 14.989 | 1.00 | 29.66 |
| ATOM | 3822 | C | PRO | 700 | 42.574 | 6.208 | 14.279 | 1.00 | 29.65 |
| ATOM | 3823 | O | PRO | 700 | 43.032 | 7.062 | 13.527 | 1.00 | 30.44 |
| ATOM | 3824 | N | TYR | 701 | 41.306 | 6.190 | 14.660 | 1.00 | 30.37 |
| ATOM | 3825 | CA | TYR | 701 | 40.359 | 7.272 | 14.367 | 1.00 | 30.01 |
| ATOM | 3826 | CB | TYR | 701 | 40.655 | 8.474 | 15.269 | 1.00 | 35.19 |
| ATOM | 3827 | CG | TYR | 701 | 40.452 | 8.215 | 16.749 | 1.00 | 39.32 |
| ATOM | 3828 | CD1 | TYR | 701 | 41.452 | 8.518 | 17.675 | 1.00 | 43.08 |
| ATOM | 3829 | CE1 | TYR | 701 | 41.258 | 8.305 | 19.041 | 1.00 | 46.20 |
| ATOM | 3830 | CD2 | TYR | 701 | 39.256 | 7.688 | 17.229 | 1.00 | 40.66 |
| ATOM | 3831 | CE2 | TYR | 701 | 39.060 | 7.469 | 18.584 | 1.00 | 43.51 |
| ATOM | 3832 | CZ | TYR | 701 | 40.056 | 7.782 | 19.485 | 1.00 | 45.75 |
| ATOM | 3833 | OH | TYR | 701 | 39.847 | 7.592 | 20.837 | 1.00 | 50.92 |
| ATOM | 3834 | C | TYR | 701 | 40.273 | 7.722 | 12.909 | 1.00 | 29.04 |
| ATOM | 3835 | O | TYR | 701 | 40.393 | 8.904 | 12.611 | 1.00 | 28.53 |
| ATOM | 3836 | N | PRO | 702 | 40.015 | 6.777 | 11.986 | 1.00 | 28.69 |
| ATOM | 3837 | CD | PRO | 702 | 39.761 | 5.346 | 12.186 | 1.00 | 26.94 |
| ATOM | 3838 | CA | PRO | 702 | 39.920 | 7.145 | 10.569 | 1.00 | 27.55 |
| ATOM | 3839 | CB | PRO | 702 | 39.709 | 5.800 | 9.882 | 1.00 | 27.91 |
| ATOM | 3840 | CG | PRO | 702 | 39.054 | 4.971 | 10.917 | 1.00 | 29.04 |
| ATOM | 3841 | C | PRO | 702 | 38.790 | 8.117 | 10.264 | 1.00 | 29.20 |
| ATOM | 3842 | O | PRO | 702 | 37.631 | 7.880 | 10.617 | 1.00 | 32.39 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3843 | N | GLY | 703 | 39.148 | 9.213 | 9.591 | 1.00 | 28.34 |
| ATOM | 3844 | CA | GLY | 703 | 38.191 | 10.236 | 9.226 | 1.00 | 25.97 |
| ATOM | 3845 | C | GLY | 703 | 37.960 | 11.289 | 10.297 | 1.00 | 28.00 |
| ATOM | 3846 | O | GLY | 703 | 37.175 | 12.213 | 10.079 | 1.00 | 26.40 |
| ATOM | 3847 | N | VAL | 704 | 38.621 | 11.139 | 11.448 | 1.00 | 29.54 |
| ATOM | 3848 | CA | VAL | 704 | 38.480 | 12.061 | 12.576 | 1.00 | 30.61 |
| ATOM | 3849 | CB | VAL | 704 | 38.606 | 11.324 | 13.944 | 1.00 | 32.54 |
| ATOM | 3850 | CG1 | VAL | 704 | 38.577 | 12.324 | 15.111 | 1.00 | 31.95 |
| ATOM | 3851 | CG2 | VAL | 704 | 37.482 | 10.311 | 14.103 | 1.00 | 34.62 |
| ATOM | 3852 | C | VAL | 704 | 39.490 | 13.210 | 12.557 | 1.00 | 31.37 |
| ATOM | 3853 | O | VAL | 704 | 40.683 | 13.001 | 12.757 | 1.00 | 31.73 |
| ATOM | 3854 | N | PRO | 705 | 39.030 | 14.430 | 12.281 | 1.00 | 32.70 |
| ATOM | 3855 | CD | PRO | 705 | 37.669 | 14.770 | 11.819 | 1.00 | 33.75 |
| ATOM | 3856 | CA | PRO | 705 | 39.910 | 15.599 | 12.243 | 1.00 | 31.90 |
| ATOM | 3857 | CB | PRO | 705 | 39.065 | 16.641 | 11.518 | 1.00 | 32.66 |
| ATOM | 3858 | CG | PRO | 705 | 37.674 | 16.273 | 11.906 | 1.00 | 35.32 |
| ATOM | 3859 | C | PRO | 705 | 40.331 | 16.053 | 13.635 | 1.00 | 31.85 |
| ATOM | 3860 | O | PRO | 705 | 39.709 | 15.686 | 14.634 | 1.00 | 31.50 |
| ATOM | 3861 | N | VAL | 706 | 41.372 | 16.879 | 13.676 | 1.00 | 32.32 |
| ATOM | 3862 | CA | VAL | 706 | 41.945 | 17.389 | 14.925 | 1.00 | 36.88 |
| ATOM | 3863 | CB | VAL | 706 | 42.991 | 18.505 | 14.664 | 1.00 | 39.77 |
| ATOM | 3864 | CG1 | VAL | 706 | 43.657 | 18.907 | 15.974 | 1.00 | 39.17 |
| ATOM | 3865 | CG2 | VAL | 706 | 44.035 | 18.057 | 13.618 | 1.00 | 38.70 |
| ATOM | 3866 | C | VAL | 706 | 40.938 | 17.923 | 15.953 | 1.00 | 37.80 |
| ATOM | 3867 | O | VAL | 706 | 40.994 | 17.581 | 17.140 | 1.00 | 37.45 |
| ATOM | 3868 | N | GLU | 707 | 39.991 | 18.724 | 15.483 | 1.00 | 38.19 |
| ATOM | 3869 | CA | GLU | 707 | 39.009 | 19.308 | 16.370 | 1.00 | 37.31 |
| ATOM | 3870 | CB | GLU | 707 | 38.208 | 20.361 | 15.619 | 1.00 | 37.46 |
| ATOM | 3871 | C | GLU | 707 | 38.084 | 18.264 | 16.994 | 1.00 | 39.56 |
| ATOM | 3872 | O | GLU | 707 | 37.739 | 18.344 | 18.177 | 1.00 | 41.39 |
| ATOM | 3873 | N | GLU | 708 | 37.724 | 17.260 | 16.206 | 1.00 | 39.99 |
| ATOM | 3874 | CA | GLU | 708 | 36.840 | 16.212 | 16.684 | 1.00 | 40.08 |
| ATOM | 3875 | CB | GLU | 708 | 36.334 | 15.377 | 15.515 | 1.00 | 43.96 |
| ATOM | 3876 | CG | GLU | 708 | 35.505 | 16.163 | 14.496 | 1.00 | 46.61 |
| ATOM | 3877 | CD | GLU | 708 | 34.288 | 16.851 | 15.099 | 1.00 | 52.77 |
| ATOM | 3878 | OE1 | GLU | 708 | 33.659 | 16.305 | 16.040 | 1.00 | 52.52 |
| ATOM | 3879 | OE2 | GLU | 708 | 33.954 | 17.955 | 14.604 | 1.00 | 57.04 |
| ATOM | 3880 | C | GLU | 708 | 37.551 | 15.337 | 17.704 | 1.00 | 39.89 |
| ATOM | 3881 | O | GLU | 708 | 36.944 | 14.900 | 18.684 | 1.00 | 39.47 |
| ATOM | 3882 | N | LEU | 709 | 38.838 | 15.086 | 17.471 | 1.00 | 38.99 |
| ATOM | 3883 | CA | LEU | 709 | 39.638 | 14.277 | 18.393 | 1.00 | 37.51 |
| ATOM | 3884 | CB | LEU | 709 | 41.079 | 14.120 | 17.892 | 1.00 | 34.15 |
| ATOM | 3885 | CG | LEU | 709 | 42.061 | 13.338 | 18.787 | 1.00 | 30.94 |
| ATOM | 3886 | CD1 | LEU | 709 | 41.861 | 11.834 | 18.689 | 1.00 | 28.48 |
| ATOM | 3887 | CD2 | LEU | 709 | 43.459 | 13.712 | 18.395 | 1.00 | 29.02 |
| ATOM | 3888 | C | LEU | 709 | 39.644 | 14.961 | 19.751 | 1.00 | 38.18 |
| ATOM | 3889 | O | LEU | 709 | 39.460 | 14.313 | 20.787 | 1.00 | 38.08 |
| ATOM | 3890 | N | PHE | 710 | 39.833 | 16.276 | 19.749 | 1.00 | 39.68 |
| ATOM | 3891 | CA | PHE | 710 | 39.845 | 17.021 | 21.001 | 1.00 | 43.27 |
| ATOM | 3892 | CB | PHE | 710 | 40.024 | 18.524 | 20.747 | 1.00 | 43.66 |
| ATOM | 3893 | CG | PHE | 710 | 41.376 | 18.888 | 20.225 | 1.00 | 46.36 |
| ATOM | 3894 | CD1 | PHE | 710 | 42.459 | 18.024 | 20.403 | 1.00 | 48.33 |

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ATOM    3895  CD2  PHE    710        41.579  20.084  19.544  1.00 47.76
ATOM    3896  CE1  PHE    710        43.723  18.343  19.915  1.00 51.79
ATOM    3897  CE2  PHE    710        42.839  20.417  19.046  1.00 50.36
ATOM    3898  CZ   PHE    710        43.916  19.544  19.233  1.00 53.02
ATOM    3899  C    PHE    710        38.558  16.746  21.758  1.00 44.74
ATOM    3900  O    PHE    710        38.587  16.422  22.952  1.00 44.99
ATOM    3901  N    LYS    711        37.445  16.777  21.032  1.00 45.27
ATOM    3902  CA   LYS    711        36.146  16.529  21.627  1.00 44.00
ATOM    3903  CB   LYS    711        35.031  16.870  20.634  1.00 46.68
ATOM    3904  CG   LYS    711        33.645  16.758  21.235  1.00 52.36
ATOM    3905  CD   LYS    711        32.556  17.224  20.293  1.00 54.43
ATOM    3906  CE   LYS    711        31.197  16.809  20.826  1.00 55.93
ATOM    3907  NZ   LYS    711        30.101  17.220  19.912  1.00 63.51
ATOM    3908  C    LYS    711        36.052  15.078  22.120  1.00 42.15
ATOM    3909  O    LYS    711        35.635  14.827  23.250  1.00 40.85
ATOM    3910  N    LEU    712        36.467  14.125  21.294  1.00 40.98
ATOM    3911  CA   LEU    712        36.432  12.719  21.691  1.00 42.26
ATOM    3912  CB   LEU    712        37.012  11.814  20.597  1.00 39.67
ATOM    3913  CG   LEU    712        36.159  11.449  19.381  1.00 39.06
ATOM    3914  CD1  LEU    712        36.899  10.440  18.504  1.00 36.97
ATOM    3915  CD2  LEU    712        34.842  10.868  19.857  1.00 36.48
ATOM    3916  C    LEU    712        37.232  12.513  22.974  1.00 43.61
ATOM    3917  O    LEU    712        36.796  11.785  23.875  1.00 44.10
ATOM    3918  N    LEU    713        38.407  13.141  23.038  1.00 43.57
ATOM    3919  CA   LEU    713        39.271  13.034  24.207  1.00 43.67
ATOM    3920  CB   LEU    713        40.619  13.726  23.958  1.00 42.24
ATOM    3921  CG   LEU    713        41.569  13.004  22.989  1.00 38.81
ATOM    3922  CD1  LEU    713        42.856  13.796  22.817  1.00 30.86
ATOM    3923  CD2  LEU    713        41.873  11.591  23.519  1.00 34.27
ATOM    3924  C    LEU    713        38.589  13.594  25.450  1.00 44.78
ATOM    3925  O    LEU    713        38.548  12.919  26.472  1.00 46.04
ATOM    3926  N    LYS    714        38.002  14.785  25.344  1.00 44.72
ATOM    3927  CA   LYS    714        37.304  15.394  26.471  1.00 44.34
ATOM    3928  CB   LYS    714        36.818  16.799  26.114  1.00 43.76
ATOM    3929  CG   LYS    714        37.955  17.761  25.926  1.00 46.37
ATOM    3930  CD   LYS    714        37.497  19.174  25.628  1.00 52.22
ATOM    3931  CE   LYS    714        38.701  20.044  25.235  1.00 57.37
ATOM    3932  NZ   LYS    714        39.792  20.059  26.279  1.00 58.02
ATOM    3933  C    LYS    714        36.142  14.534  26.972  1.00 44.17
ATOM    3934  O    LYS    714        35.861  14.499  28.167  1.00 45.14
ATOM    3935  N    GLU    715        35.498  13.809  26.068  1.00 43.86
ATOM    3936  CA   GLU    715        34.392  12.935  26.430  1.00 42.94
ATOM    3937  CB   GLU    715        33.518  12.652  25.195  1.00 46.57
ATOM    3938  CG   GLU    715        32.930  13.897  24.532  1.00 51.37
ATOM    3939  CD   GLU    715        32.032  13.571  23.338  1.00 54.24
ATOM    3940  OE1  GLU    715        32.215  12.503  22.704  1.00 54.19
ATOM    3941  OE2  GLU    715        31.139  14.392  23.033  1.00 55.01
ATOM    3942  C    GLU    715        34.878  11.607  27.036  1.00 41.36
ATOM    3943  O    GLU    715        34.076  10.730  27.348  1.00 38.24
ATOM    3944  N    GLY    716        36.184  11.452  27.182  1.00 41.41
ATOM    3945  CA   GLY    716        36.727  10.225  27.737  1.00 41.78
ATOM    3946  C    GLY    716        36.602   9.034  26.799  1.00 42.65
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3947 | O | GLY | 716 | 36.661 | 7.874 | 27.225 | 1.00 | 41.41 |
| ATOM | 3948 | N | HIS | 717 | 36.439 | 9.321 | 25.513 | 1.00 | 44.56 |
| ATOM | 3949 | CA | HIS | 717 | 36.286 | 8.291 | 24.502 | 1.00 | 45.91 |
| ATOM | 3950 | CB | HIS | 717 | 35.935 | 8.926 | 23.153 | 1.00 | 46.65 |
| ATOM | 3951 | CG | HIS | 717 | 35.860 | 7.946 | 22.024 | 1.00 | 50.03 |
| ATOM | 3952 | CD2 | HIS | 717 | 34.842 | 7.171 | 21.581 | 1.00 | 49.92 |
| ATOM | 3953 | ND1 | HIS | 717 | 36.946 | 7.634 | 21.235 | 1.00 | 51.38 |
| ATOM | 3954 | CE1 | HIS | 717 | 36.604 | 6.708 | 20.360 | 1.00 | 50.10 |
| ATOM | 3955 | NE2 | HIS | 717 | 35.335 | 6.408 | 20.550 | 1.00 | 49.34 |
| ATOM | 3956 | C | HIS | 717 | 37.535 | 7.434 | 24.354 | 1.00 | 47.68 |
| ATOM | 3957 | O | HIS | 717 | 38.649 | 7.949 | 24.287 | 1.00 | 49.77 |
| ATOM | 3958 | N | ARG | 718 | 37.328 | 6.118 | 24.283 | 1.00 | 48.18 |
| ATOM | 3959 | CA | ARG | 718 | 38.403 | 5.148 | 24.116 | 1.00 | 46.95 |
| ATOM | 3960 | CB | ARG | 718 | 38.571 | 4.307 | 25.385 | 1.00 | 45.75 |
| ATOM | 3961 | CG | ARG | 718 | 38.945 | 5.125 | 26.618 | 1.00 | 47.15 |
| ATOM | 3962 | CD | ARG | 718 | 40.273 | 5.852 | 26.420 | 1.00 | 46.61 |
| ATOM | 3963 | NE | ARG | 718 | 40.722 | 6.579 | 27.608 | 1.00 | 45.57 |
| ATOM | 3964 | CZ | ARG | 718 | 40.601 | 7.896 | 27.779 | 1.00 | 45.48 |
| ATOM | 3965 | NH1 | ARG | 718 | 40.033 | 8.644 | 26.845 | 1.00 | 44.14 |
| ATOM | 3966 | NH2 | ARG | 718 | 41.122 | 8.480 | 28.854 | 1.00 | 43.32 |
| ATOM | 3967 | C | ARG | 718 | 38.109 | 4.250 | 22.912 | 1.00 | 47.56 |
| ATOM | 3968 | O | ARG | 718 | 36.946 | 3.991 | 22.589 | 1.00 | 48.37 |
| ATOM | 3969 | N | MET | 719 | 39.149 | 3.873 | 22.181 | 1.00 | 47.33 |
| ATOM | 3970 | CA | MET | 719 | 38.984 | 3.021 | 21.013 | 1.00 | 47.90 |
| ATOM | 3971 | CB | MET | 719 | 40.282 | 2.939 | 20.198 | 1.00 | 47.21 |
| ATOM | 3972 | CG | MET | 719 | 40.652 | 4.245 | 19.509 | 1.00 | 45.79 |
| ATOM | 3973 | SD | MET | 719 | 42.095 | 4.104 | 18.440 | 1.00 | 42.81 |
| ATOM | 3974 | CE | MET | 719 | 43.377 | 3.970 | 19.604 | 1.00 | 43.02 |
| ATOM | 3975 | C | MET | 719 | 38.519 | 1.629 | 21.392 | 1.00 | 49.99 |
| ATOM | 3976 | O | MET | 719 | 38.889 | 1.102 | 22.450 | 1.00 | 47.98 |
| ATOM | 3977 | N | ASP | 720 | 37.690 | 1.050 | 20.523 | 1.00 | 53.40 |
| ATOM | 3978 | CA | ASP | 720 | 37.135 | -0.288 | 20.722 | 1.00 | 53.19 |
| ATOM | 3979 | CB | ASP | 720 | 36.089 | -0.638 | 19.647 | 1.00 | 56.95 |
| ATOM | 3980 | CG | ASP | 720 | 34.916 | 0.333 | 19.605 | 1.00 | 61.65 |
| ATOM | 3981 | OD1 | ASP | 720 | 34.908 | 1.331 | 20.356 | 1.00 | 68.60 |
| ATOM | 3982 | OD2 | ASP | 720 | 33.996 | 0.095 | 18.792 | 1.00 | 61.19 |
| ATOM | 3983 | C | ASP | 720 | 38.208 | -1.372 | 20.713 | 1.00 | 51.12 |
| ATOM | 3984 | O | ASP | 720 | 39.263 | -1.229 | 20.081 | 1.00 | 50.71 |
| ATOM | 3985 | N | LYS | 721 | 37.926 | -2.453 | 21.432 | 1.00 | 48.85 |
| ATOM | 3986 | CA | LYS | 721 | 38.833 | -3.576 | 21.509 | 1.00 | 47.92 |
| ATOM | 3987 | CB | LYS | 721 | 38.335 | -4.560 | 22.562 | 1.00 | 47.79 |
| ATOM | 3988 | CG | LYS | 721 | 39.024 | -5.901 | 22.521 | 1.00 | 51.08 |
| ATOM | 3989 | CD | LYS | 721 | 38.493 | -6.810 | 23.597 | 1.00 | 53.21 |
| ATOM | 3990 | CE | LYS | 721 | 38.484 | -8.255 | 23.141 | 1.00 | 54.60 |
| ATOM | 3991 | NZ | LYS | 721 | 38.158 | -9.176 | 24.268 | 1.00 | 61.37 |
| ATOM | 3992 | C | LYS | 721 | 38.861 | -4.261 | 20.155 | 1.00 | 49.01 |
| ATOM | 3993 | O | LYS | 721 | 37.822 | -4.688 | 19.653 | 1.00 | 52.79 |
| ATOM | 3994 | N | PRO | 722 | 40.053 | -4.366 | 19.541 | 1.00 | 48.92 |
| ATOM | 3995 | CD | PRO | 722 | 41.356 | -3.839 | 19.972 | 1.00 | 51.11 |
| ATOM | 3996 | CA | PRO | 722 | 40.167 | -5.011 | 18.233 | 1.00 | 46.01 |
| ATOM | 3997 | CB | PRO | 722 | 41.663 | -4.904 | 17.918 | 1.00 | 45.64 |
| ATOM | 3998 | CG | PRO | 722 | 42.090 | -3.690 | 18.646 | 1.00 | 47.86 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 3999 | C | PRO | 722 | 39.745 | -6.466 | 18.303 | 1.00 | 43.57 |
| ATOM | 4000 | O | PRO | 722 | 39.719 | -7.069 | 19.381 | 1.00 | 41.72 |
| ATOM | 4001 | N | SER | 723 | 39.360 | -7.001 | 17.150 | 1.00 | 43.14 |
| ATOM | 4002 | CA | SER | 723 | 38.991 | -8.398 | 17.044 | 1.00 | 41.85 |
| ATOM | 4003 | CB | SER | 723 | 38.260 | -8.660 | 15.734 | 1.00 | 37.27 |
| ATOM | 4004 | OG | SER | 723 | 39.112 | -8.421 | 14.639 | 1.00 | 39.44 |
| ATOM | 4005 | C | SER | 723 | 40.339 | -9.110 | 17.049 | 1.00 | 41.68 |
| ATOM | 4006 | O | SER | 723 | 41.299 | -8.605 | 16.493 | 1.00 | 40.84 |
| ATOM | 4007 | N | ASN | 724 | 40.405 | -10.275 | 17.683 | 1.00 | 45.99 |
| ATOM | 4008 | CA | ASN | 724 | 41.651 | -11.034 | 17.800 | 1.00 | 49.22 |
| ATOM | 4009 | CB | ASN | 724 | 42.342 | -11.215 | 16.453 | 1.00 | 52.35 |
| ATOM | 4010 | CG | ASN | 724 | 41.768 | -12.357 | 15.668 | 1.00 | 58.07 |
| ATOM | 4011 | OD1 | ASN | 724 | 41.821 | -13.506 | 16.103 | 1.00 | 62.42 |
| ATOM | 4012 | ND2 | ASN | 724 | 41.186 | -12.054 | 14.513 | 1.00 | 62.13 |
| ATOM | 4013 | C | ASN | 724 | 42.558 | -10.323 | 18.787 | 1.00 | 49.77 |
| ATOM | 4014 | O | ASN | 724 | 43.698 | -9.982 | 18.494 | 1.00 | 51.48 |
| ATOM | 4015 | N | CYS | 725 | 41.995 | -10.054 | 19.954 | 1.00 | 50.34 |
| ATOM | 4016 | CA | CYS | 725 | 42.698 | -9.398 | 21.028 | 1.00 | 49.83 |
| ATOM | 4017 | CB | CYS | 725 | 42.623 | -7.878 | 20.868 | 1.00 | 47.11 |
| ATOM | 4018 | SG | CYS | 725 | 43.485 | -6.992 | 22.169 | 1.00 | 38.55 |
| ATOM | 4019 | C | CYS | 725 | 42.001 | -9.861 | 22.299 | 1.00 | 50.11 |
| ATOM | 4020 | O | CYS | 725 | 40.772 | -9.852 | 22.383 | 1.00 | 50.63 |
| ATOM | 4021 | N | THR | 726 | 42.788 | -10.350 | 23.244 | 1.00 | 50.37 |
| ATOM | 4022 | CA | THR | 726 | 42.261 | -10.843 | 24.497 | 1.00 | 51.05 |
| ATOM | 4023 | CB | THR | 726 | 43.341 | -11.663 | 25.234 | 1.00 | 53.50 |
| ATOM | 4024 | OG1 | THR | 726 | 44.292 | -10.780 | 25.829 | 1.00 | 57.56 |
| ATOM | 4025 | CG2 | THR | 726 | 44.074 | -12.554 | 24.241 | 1.00 | 52.55 |
| ATOM | 4026 | C | THR | 726 | 41.843 | -9.665 | 25.354 | 1.00 | 52.18 |
| ATOM | 4027 | O | THR | 726 | 42.403 | -8.574 | 25.219 | 1.00 | 55.14 |
| ATOM | 4028 | N | ASN | 727 | 40.868 | -9.860 | 26.237 | 1.00 | 52.55 |
| ATOM | 4029 | CA | ASN | 727 | 40.401 | -8.781 | 27.114 | 1.00 | 53.17 |
| ATOM | 4030 | CB | ASN | 727 | 39.246 | -9.265 | 27.992 | 1.00 | 60.65 |
| ATOM | 4031 | CG | ASN | 727 | 39.584 | -10.545 | 28.751 | 1.00 | 68.99 |
| ATOM | 4032 | OD1 | ASN | 727 | 40.704 | -10.718 | 29.243 | 1.00 | 73.66 |
| ATOM | 4033 | ND2 | ASN | 727 | 38.629 | -11.454 | 28.825 | 1.00 | 74.66 |
| ATOM | 4034 | C | ASN | 727 | 41.537 | -8.254 | 27.976 | 1.00 | 50.79 |
| ATOM | 4035 | O | ASN | 727 | 41.513 | -7.107 | 28.414 | 1.00 | 48.17 |
| ATOM | 4036 | N | GLU | 728 | 42.527 | -9.111 | 28.215 | 1.00 | 50.18 |
| ATOM | 4037 | CA | GLU | 728 | 43.693 | -8.764 | 29.020 | 1.00 | 49.68 |
| ATOM | 4038 | CB | GLU | 728 | 44.544 | -10.011 | 29.289 | 1.00 | 50.61 |
| ATOM | 4039 | CG | GLU | 728 | 45.801 | -9.758 | 30.120 | 1.00 | 55.44 |
| ATOM | 4040 | CD | GLU | 728 | 46.509 | -11.045 | 30.542 | 1.00 | 56.45 |
| ATOM | 4041 | OE1 | GLU | 728 | 46.737 | -11.930 | 29.685 | 1.00 | 53.73 |
| ATOM | 4042 | OE2 | GLU | 728 | 46.865 | -11.161 | 31.733 | 1.00 | 57.38 |
| ATOM | 4043 | C | GLU | 728 | 44.509 | -7.713 | 28.272 | 1.00 | 46.92 |
| ATOM | 4044 | O | GLU | 728 | 44.760 | -6.614 | 28.785 | 1.00 | 46.08 |
| ATOM | 4045 | N | LEU | 729 | 44.869 | -8.039 | 27.033 | 1.00 | 42.69 |
| ATOM | 4046 | CA | LEU | 729 | 45.641 | -7.137 | 26.192 | 1.00 | 40.42 |
| ATOM | 4047 | CB | LEU | 729 | 45.950 | -7.796 | 24.846 | 1.00 | 34.84 |
| ATOM | 4048 | CG | LEU | 729 | 47.004 | -8.900 | 24.952 | 1.00 | 34.35 |
| ATOM | 4049 | CD1 | LEU | 729 | 46.960 | -9.780 | 23.749 | 1.00 | 31.03 |
| ATOM | 4050 | CD2 | LEU | 729 | 48.404 | -8.320 | 25.139 | 1.00 | 33.63 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4051 | C | LEU | 729 | 44.909 | -5.817 | 25.985 | 1.00 | 40.58 |
| ATOM | 4052 | O | LEU | 729 | 45.524 | -4.760 | 25.929 | 1.00 | 40.10 |
| ATOM | 4053 | N | TYR | 730 | 43.591 | -5.886 | 25.917 | 1.00 | 39.32 |
| ATOM | 4054 | CA | TYR | 730 | 42.807 | -4.694 | 25.720 | 1.00 | 41.49 |
| ATOM | 4055 | CB | TYR | 730 | 41.384 | -5.052 | 25.302 | 1.00 | 39.70 |
| ATOM | 4056 | CG | TYR | 730 | 40.507 | -3.846 | 25.099 | 1.00 | 39.53 |
| ATOM | 4057 | CD1 | TYR | 730 | 40.828 | -2.879 | 24.142 | 1.00 | 35.10 |
| ATOM | 4058 | CE1 | TYR | 730 | 40.019 | -1.758 | 23.958 | 1.00 | 36.33 |
| ATOM | 4059 | CD2 | TYR | 730 | 39.352 | -3.661 | 25.874 | 1.00 | 38.44 |
| ATOM | 4060 | CE2 | TYR | 730 | 38.537 | -2.541 | 25.696 | 1.00 | 37.68 |
| ATOM | 4061 | CZ | TYR | 730 | 38.876 | -1.601 | 24.730 | 1.00 | 36.85 |
| ATOM | 4062 | OH | TYR | 730 | 38.041 | -0.541 | 24.489 | 1.00 | 40.58 |
| ATOM | 4063 | C | TYR | 730 | 42.814 | -3.849 | 26.993 | 1.00 | 43.50 |
| ATOM | 4064 | O | TYR | 730 | 42.880 | -2.621 | 26.931 | 1.00 | 44.45 |
| ATOM | 4065 | N | MET | 731 | 42.753 | -4.492 | 28.151 | 1.00 | 46.53 |
| ATOM | 4066 | CA | MET | 731 | 42.782 | -3.744 | 29.406 | 1.00 | 48.67 |
| ATOM | 4067 | CB | MET | 731 | 42.488 | -4.668 | 30.590 | 1.00 | 54.90 |
| ATOM | 4068 | CG | MET | 731 | 41.072 | -5.229 | 30.577 | 1.00 | 63.75 |
| ATOM | 4069 | SD | MET | 731 | 39.766 | -3.998 | 30.763 | 1.00 | 69.82 |
| ATOM | 4070 | CE | MET | 731 | 39.849 | -3.788 | 32.581 | 1.00 | 68.20 |
| ATOM | 4071 | C | MET | 731 | 44.148 | -3.087 | 29.551 | 1.00 | 45.73 |
| ATOM | 4072 | O | MET | 731 | 44.273 | -2.024 | 30.160 | 1.00 | 42.09 |
| ATOM | 4073 | N | MET | 732 | 45.168 | -3.728 | 28.986 | 1.00 | 43.47 |
| ATOM | 4074 | CA | MET | 732 | 46.519 | -3.189 | 29.024 | 1.00 | 43.85 |
| ATOM | 4075 | CB | MET | 732 | 47.515 | -4.154 | 28.365 | 1.00 | 40.67 |
| ATOM | 4076 | CG | MET | 732 | 48.966 | -3.646 | 28.369 | 1.00 | 39.96 |
| ATOM | 4077 | SD | MET | 732 | 50.252 | -4.870 | 27.887 | 1.00 | 35.34 |
| ATOM | 4078 | CE | MET | 732 | 50.523 | -5.667 | 29.390 | 1.00 | 35.15 |
| ATOM | 4079 | C | MET | 732 | 46.460 | -1.860 | 28.275 | 1.00 | 43.91 |
| ATOM | 4080 | O | MET | 732 | 46.924 | -0.835 | 28.782 | 1.00 | 47.29 |
| ATOM | 4081 | N | MET | 733 | 45.798 | -1.860 | 27.120 | 1.00 | 42.51 |
| ATOM | 4082 | CA | MET | 733 | 45.639 | -0.652 | 26.319 | 1.00 | 39.85 |
| ATOM | 4083 | CB | MET | 733 | 44.888 | -0.932 | 25.013 | 1.00 | 38.08 |
| ATOM | 4084 | CG | MET | 733 | 45.614 | -1.805 | 23.991 | 1.00 | 37.14 |
| ATOM | 4085 | SD | MET | 733 | 44.509 | -2.170 | 22.578 | 1.00 | 37.32 |
| ATOM | 4086 | CE | MET | 733 | 45.198 | -3.684 | 21.929 | 1.00 | 28.98 |
| ATOM | 4087 | C | MET | 733 | 44.838 | 0.363 | 27.123 | 1.00 | 41.12 |
| ATOM | 4088 | O | MET | 733 | 45.228 | 1.532 | 27.213 | 1.00 | 44.38 |
| ATOM | 4089 | N | ARG | 734 | 43.737 | -0.084 | 27.731 | 1.00 | 40.28 |
| ATOM | 4090 | CA | ARG | 734 | 42.893 | 0.813 | 28.516 | 1.00 | 40.23 |
| ATOM | 4091 | CB | ARG | 734 | 41.632 | 0.095 | 29.007 | 1.00 | 39.95 |
| ATOM | 4092 | CG | ARG | 734 | 40.723 | -0.384 | 27.894 | 1.00 | 36.41 |
| ATOM | 4093 | CD | ARG | 734 | 40.323 | 0.741 | 26.995 | 1.00 | 39.31 |
| ATOM | 4094 | NE | ARG | 734 | 39.510 | 1.733 | 27.682 | 1.00 | 48.97 |
| ATOM | 4095 | CZ | ARG | 734 | 38.182 | 1.681 | 27.774 | 1.00 | 53.99 |
| ATOM | 4096 | NH1 | ARG | 734 | 37.503 | 0.681 | 27.222 | 1.00 | 56.64 |
| ATOM | 4097 | NH2 | ARG | 734 | 37.526 | 2.633 | 28.416 | 1.00 | 56.79 |
| ATOM | 4098 | C | ARG | 734 | 43.694 | 1.387 | 29.675 | 1.00 | 39.38 |
| ATOM | 4099 | O | ARG | 734 | 43.538 | 2.564 | 30.010 | 1.00 | 41.82 |
| ATOM | 4100 | N | ASP | 735 | 44.583 | 0.572 | 30.244 | 1.00 | 37.67 |
| ATOM | 4101 | CA | ASP | 735 | 45.465 | 1.000 | 31.339 | 1.00 | 39.58 |
| ATOM | 4102 | CB | ASP | 735 | 46.392 | -0.137 | 31.773 | 1.00 | 42.90 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4103 | CG | ASP | 735 | 45.690 | -1.175 | 32.604 | 1.00 | 47.78 |
| ATOM | 4104 | OD1 | ASP | 735 | 46.116 | -2.355 | 32.524 | 1.00 | 47.92 |
| ATOM | 4105 | OD2 | ASP | 735 | 44.733 | -0.803 | 33.339 | 1.00 | 46.75 |
| ATOM | 4106 | C | ASP | 735 | 46.339 | 2.161 | 30.881 | 1.00 | 37.68 |
| ATOM | 4107 | O | ASP | 735 | 46.447 | 3.178 | 31.579 | 1.00 | 36.83 |
| ATOM | 4108 | N | CYS | 736 | 46.996 | 1.967 | 29.734 | 1.00 | 35.06 |
| ATOM | 4109 | CA | CYS | 736 | 47.858 | 2.979 | 29.140 | 1.00 | 32.91 |
| ATOM | 4110 | CB | CYS | 736 | 48.499 | 2.469 | 27.848 | 1.00 | 27.65 |
| ATOM | 4111 | SG | CYS | 736 | 49.631 | 1.067 | 27.989 | 1.00 | 31.08 |
| ATOM | 4112 | C | CYS | 736 | 47.054 | 4.232 | 28.828 | 1.00 | 35.28 |
| ATOM | 4113 | O | CYS | 736 | 47.595 | 5.334 | 28.810 | 1.00 | 35.52 |
| ATOM | 4114 | N | TRP | 737 | 45.742 | 4.078 | 28.677 | 1.00 | 38.73 |
| ATOM | 4115 | CA | TRP | 737 | 44.885 | 5.217 | 28.352 | 1.00 | 41.10 |
| ATOM | 4116 | CB | TRP | 737 | 43.890 | 4.816 | 27.266 | 1.00 | 41.22 |
| ATOM | 4117 | CG | TRP | 737 | 44.535 | 4.362 | 25.994 | 1.00 | 40.65 |
| ATOM | 4118 | CD2 | TRP | 737 | 43.976 | 3.465 | 25.026 | 1.00 | 41.90 |
| ATOM | 4119 | CE2 | TRP | 737 | 44.932 | 3.325 | 23.990 | 1.00 | 41.02 |
| ATOM | 4120 | CE3 | TRP | 737 | 42.763 | 2.764 | 24.930 | 1.00 | 40.44 |
| ATOM | 4121 | CD1 | TRP | 737 | 45.766 | 4.721 | 25.517 | 1.00 | 39.14 |
| ATOM | 4122 | NE1 | TRP | 737 | 46.011 | 4.103 | 24.316 | 1.00 | 37.93 |
| ATOM | 4123 | CZ2 | TRP | 737 | 44.708 | 2.512 | 22.875 | 1.00 | 40.92 |
| ATOM | 4124 | CZ3 | TRP | 737 | 42.549 | 1.956 | 23.820 | 1.00 | 38.42 |
| ATOM | 4125 | CH2 | TRP | 737 | 43.518 | 1.837 | 22.812 | 1.00 | 36.49 |
| ATOM | 4126 | C | TRP | 737 | 44.159 | 5.847 | 29.538 | 1.00 | 41.39 |
| ATOM | 4127 | O | TRP | 737 | 43.163 | 6.551 | 29.366 | 1.00 | 40.86 |
| ATOM | 4128 | N | HIS | 738 | 44.685 | 5.643 | 30.743 | 1.00 | 43.61 |
| ATOM | 4129 | CA | HIS | 738 | 44.059 | 6.197 | 31.941 | 1.00 | 44.35 |
| ATOM | 4130 | CB | HIS | 738 | 44.698 | 5.596 | 33.183 | 1.00 | 45.31 |
| ATOM | 4131 | CG | HIS | 738 | 43.970 | 5.922 | 34.446 | 1.00 | 50.87 |
| ATOM | 4132 | CD2 | HIS | 738 | 43.685 | 7.111 | 35.026 | 1.00 | 49.13 |
| ATOM | 4133 | ND1 | HIS | 738 | 43.401 | 4.961 | 35.252 | 1.00 | 52.48 |
| ATOM | 4134 | CE1 | HIS | 738 | 42.798 | 5.541 | 36.275 | 1.00 | 55.70 |
| ATOM | 4135 | NE2 | HIS | 738 | 42.955 | 6.848 | 36.159 | 1.00 | 51.42 |
| ATOM | 4136 | C | HIS | 738 | 44.202 | 7.714 | 31.969 | 1.00 | 44.15 |
| ATOM | 4137 | O | HIS | 738 | 45.294 | 8.223 | 31.787 | 1.00 | 43.14 |
| ATOM | 4138 | N | ALA | 739 | 43.115 | 8.428 | 32.272 | 1.00 | 45.42 |
| ATOM | 4139 | CA | ALA | 739 | 43.141 | 9.895 | 32.318 | 1.00 | 47.29 |
| ATOM | 4140 | CB | ALA | 739 | 41.792 | 10.426 | 32.752 | 1.00 | 49.75 |
| ATOM | 4141 | C | ALA | 739 | 44.240 | 10.454 | 33.223 | 1.00 | 48.73 |
| ATOM | 4142 | O | ALA | 739 | 44.921 | 11.415 | 32.868 | 1.00 | 49.32 |
| ATOM | 4143 | N | VAL | 740 | 44.331 | 9.893 | 34.425 | 1.00 | 50.51 |
| ATOM | 4144 | CA | VAL | 740 | 45.332 | 10.262 | 35.424 | 1.00 | 51.32 |
| ATOM | 4145 | CB | VAL | 740 | 44.861 | 9.880 | 36.842 | 1.00 | 52.29 |
| ATOM | 4146 | CG1 | VAL | 740 | 45.905 | 10.254 | 37.869 | 1.00 | 53.73 |
| ATOM | 4147 | CG2 | VAL | 740 | 43.551 | 10.575 | 37.152 | 1.00 | 53.54 |
| ATOM | 4148 | C | VAL | 740 | 46.656 | 9.535 | 35.121 | 1.00 | 51.06 |
| ATOM | 4149 | O | VAL | 740 | 46.780 | 8.320 | 35.348 | 1.00 | 50.81 |
| ATOM | 4150 | N | PRO | 741 | 47.670 | 10.280 | 34.657 | 1.00 | 50.12 |
| ATOM | 4151 | CD | PRO | 741 | 47.595 | 11.738 | 34.454 | 1.00 | 50.19 |
| ATOM | 4152 | CA | PRO | 741 | 49.003 | 9.775 | 34.294 | 1.00 | 51.10 |
| ATOM | 4153 | CB | PRO | 741 | 49.790 | 11.060 | 34.024 | 1.00 | 50.35 |
| ATOM | 4154 | CG | PRO | 741 | 48.731 | 11.978 | 33.492 | 1.00 | 50.13 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4155 | C | PRO | 741 | 49.687 | 8.902 | 35.340 | 1.00 | 52.02 |
| ATOM | 4156 | O | PRO | 741 | 50.374 | 7.941 | 34.998 | 1.00 | 50.79 |
| ATOM | 4157 | N | SER | 742 | 49.482 | 9.228 | 36.613 | 1.00 | 53.75 |
| ATOM | 4158 | CA | SER | 742 | 50.079 | 8.474 | 37.708 | 1.00 | 54.58 |
| ATOM | 4159 | CB | SER | 742 | 49.921 | 9.245 | 39.020 | 1.00 | 57.25 |
| ATOM | 4160 | OG | SER | 742 | 48.572 | 9.629 | 39.237 | 1.00 | 61.69 |
| ATOM | 4161 | C | SER | 742 | 49.479 | 7.077 | 37.851 | 1.00 | 53.33 |
| ATOM | 4162 | O | SER | 742 | 50.074 | 6.189 | 38.464 | 1.00 | 52.98 |
| ATOM | 4163 | N | GLN | 743 | 48.286 | 6.897 | 37.305 | 1.00 | 52.97 |
| ATOM | 4164 | CA | GLN | 743 | 47.616 | 5.613 | 37.390 | 1.00 | 52.15 |
| ATOM | 4165 | CB | GLN | 743 | 46.108 | 5.827 | 37.505 | 1.00 | 56.12 |
| ATOM | 4166 | CG | GLN | 743 | 45.506 | 5.374 | 38.838 | 1.00 | 60.50 |
| ATOM | 4167 | CD | GLN | 743 | 46.269 | 5.887 | 40.046 | 1.00 | 64.45 |
| ATOM | 4168 | OE1 | GLN | 743 | 46.910 | 5.114 | 40.752 | 1.00 | 65.64 |
| ATOM | 4169 | NE2 | GLN | 743 | 46.199 | 7.194 | 40.290 | 1.00 | 67.99 |
| ATOM | 4170 | C | GLN | 743 | 47.963 | 4.690 | 36.229 | 1.00 | 49.54 |
| ATOM | 4171 | O | GLN | 743 | 47.629 | 3.499 | 36.246 | 1.00 | 50.07 |
| ATOM | 4172 | N | ARG | 744 | 48.605 | 5.241 | 35.202 | 1.00 | 46.93 |
| ATOM | 4173 | CA | ARG | 744 | 49.010 | 4.437 | 34.044 | 1.00 | 44.51 |
| ATOM | 4174 | CB | ARG | 744 | 49.478 | 5.330 | 32.894 | 1.00 | 39.30 |
| ATOM | 4175 | CG | ARG | 744 | 48.433 | 6.300 | 32.360 | 1.00 | 32.53 |
| ATOM | 4176 | CD | ARG | 744 | 48.991 | 7.178 | 31.254 | 1.00 | 25.50 |
| ATOM | 4177 | NE | ARG | 744 | 48.034 | 8.218 | 30.932 | 1.00 | 32.16 |
| ATOM | 4178 | CZ | ARG | 744 | 48.352 | 9.454 | 30.542 | 1.00 | 34.35 |
| ATOM | 4179 | NH1 | ARG | 744 | 49.622 | 9.814 | 30.400 | 1.00 | 30.49 |
| ATOM | 4180 | NH2 | ARG | 744 | 47.382 | 10.349 | 30.350 | 1.00 | 32.23 |
| ATOM | 4181 | C | ARG | 744 | 50.153 | 3.498 | 34.472 | 1.00 | 44.61 |
| ATOM | 4182 | O | ARG | 744 | 50.833 | 3.741 | 35.474 | 1.00 | 47.68 |
| ATOM | 4183 | N | PRO | 745 | 50.319 | 2.365 | 33.765 | 1.00 | 43.21 |
| ATOM | 4184 | CD | PRO | 745 | 49.444 | 1.737 | 32.763 | 1.00 | 42.00 |
| ATOM | 4185 | CA | PRO | 745 | 51.414 | 1.470 | 34.157 | 1.00 | 40.11 |
| ATOM | 4186 | CB | PRO | 745 | 51.004 | 0.132 | 33.532 | 1.00 | 37.54 |
| ATOM | 4187 | CG | PRO | 745 | 50.251 | 0.515 | 32.335 | 1.00 | 36.49 |
| ATOM | 4188 | C | PRO | 745 | 52.744 | 1.956 | 33.612 | 1.00 | 39.15 |
| ATOM | 4189 | O | PRO | 745 | 52.807 | 2.654 | 32.602 | 1.00 | 40.56 |
| ATOM | 4190 | N | THR | 746 | 53.812 | 1.626 | 34.316 | 1.00 | 37.77 |
| ATOM | 4191 | CA | THR | 746 | 55.135 | 2.020 | 33.886 | 1.00 | 37.61 |
| ATOM | 4192 | CB | THR | 746 | 56.113 | 2.132 | 35.091 | 1.00 | 39.14 |
| ATOM | 4193 | OG1 | THR | 746 | 56.439 | 0.824 | 35.600 | 1.00 | 35.16 |
| ATOM | 4194 | CG2 | THR | 746 | 55.489 | 2.990 | 36.195 | 1.00 | 36.82 |
| ATOM | 4195 | C | THR | 746 | 55.687 | 1.036 | 32.852 | 1.00 | 36.75 |
| ATOM | 4196 | O | THR | 746 | 55.228 | -0.103 | 32.772 | 1.00 | 32.89 |
| ATOM | 4197 | N | PHE | 747 | 56.649 | 1.482 | 32.043 | 1.00 | 36.56 |
| ATOM | 4198 | CA | PHE | 747 | 57.267 | 0.599 | 31.055 | 1.00 | 33.79 |
| ATOM | 4199 | CB | PHE | 747 | 58.305 | 1.350 | 30.226 | 1.00 | 28.85 |
| ATOM | 4200 | CG | PHE | 747 | 57.702 | 2.123 | 29.103 | 1.00 | 30.71 |
| ATOM | 4201 | CD1 | PHE | 747 | 57.060 | 1.455 | 28.059 | 1.00 | 26.42 |
| ATOM | 4202 | CD2 | PHE | 747 | 57.749 | 3.510 | 29.080 | 1.00 | 28.73 |
| ATOM | 4203 | CE1 | PHE | 747 | 56.469 | 2.154 | 27.025 | 1.00 | 26.56 |
| ATOM | 4204 | CE2 | PHE | 747 | 57.150 | 4.216 | 28.047 | 1.00 | 28.97 |
| ATOM | 4205 | CZ | PHE | 747 | 56.518 | 3.535 | 27.018 | 1.00 | 28.95 |
| ATOM | 4206 | C | PHE | 747 | 57.901 | -0.593 | 31.732 | 1.00 | 34.64 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4207 | O | PHE | 747 | 58.008 | -1.667 | 31.156 | 1.00 | 31.47 |
| ATOM | 4208 | N | LYS | 748 | 58.328 | -0.399 | 32.972 | 1.00 | 38.86 |
| ATOM | 4209 | CA | LYS | 748 | 58.920 | -1.480 | 33.727 | 1.00 | 39.79 |
| ATOM | 4210 | CB | LYS | 748 | 59.529 | -0.952 | 35.026 | 1.00 | 43.68 |
| ATOM | 4211 | CG | LYS | 748 | 60.200 | -2.047 | 35.838 | 1.00 | 48.11 |
| ATOM | 4212 | CD | LYS | 748 | 60.917 | -1.515 | 37.064 | 1.00 | 51.33 |
| ATOM | 4213 | CE | LYS | 748 | 61.353 | -2.660 | 37.973 | 1.00 | 51.17 |
| ATOM | 4214 | NZ | LYS | 748 | 62.135 | -2.141 | 39.127 | 1.00 | 56.55 |
| ATOM | 4215 | C | LYS | 748 | 57.813 | -2.503 | 34.008 | 1.00 | 41.14 |
| ATOM | 4216 | O | LYS | 748 | 58.025 | -3.706 | 33.848 | 1.00 | 38.24 |
| ATOM | 4217 | N | GLN | 749 | 56.622 | -2.008 | 34.383 | 1.00 | 41.20 |
| ATOM | 4218 | CA | GLN | 749 | 55.454 | -2.856 | 34.669 | 1.00 | 40.49 |
| ATOM | 4219 | CB | GLN | 749 | 54.254 | -2.015 | 35.134 | 1.00 | 45.70 |
| ATOM | 4220 | CG | GLN | 749 | 54.378 | -1.368 | 36.500 | 1.00 | 50.61 |
| ATOM | 4221 | CD | GLN | 749 | 53.203 | -0.441 | 36.797 | 1.00 | 55.26 |
| ATOM | 4222 | OE1 | GLN | 749 | 53.392 | 0.727 | 37.123 | 1.00 | 58.00 |
| ATOM | 4223 | NE2 | GLN | 749 | 51.988 | -0.951 | 36.665 | 1.00 | 59.25 |
| ATOM | 4224 | C | GLN | 749 | 55.049 | -3.588 | 33.397 | 1.00 | 37.42 |
| ATOM | 4225 | O | GLN | 749 | 54.964 | -4.810 | 33.369 | 1.00 | 36.00 |
| ATOM | 4226 | N | LEU | 750 | 54.810 | -2.817 | 32.340 | 1.00 | 36.76 |
| ATOM | 4227 | CA | LEU | 750 | 54.409 | -3.355 | 31.033 | 1.00 | 35.39 |
| ATOM | 4228 | CB | LEU | 750 | 54.358 | -2.241 | 29.984 | 1.00 | 30.97 |
| ATOM | 4229 | CG | LEU | 750 | 53.369 | -1.091 | 30.177 | 1.00 | 27.36 |
| ATOM | 4230 | CD1 | LEU | 750 | 53.745 | 0.037 | 29.217 | 1.00 | 29.15 |
| ATOM | 4231 | CD2 | LEU | 750 | 51.941 | -1.578 | 29.934 | 1.00 | 29.22 |
| ATOM | 4232 | C | LEU | 750 | 55.369 | -4.437 | 30.557 | 1.00 | 35.16 |
| ATOM | 4233 | O | LEU | 750 | 54.934 | -5.449 | 30.014 | 1.00 | 34.45 |
| ATOM | 4234 | N | VAL | 751 | 56.673 | -4.212 | 30.721 | 1.00 | 38.76 |
| ATOM | 4235 | CA | VAL | 751 | 57.656 | -5.217 | 30.312 | 1.00 | 38.69 |
| ATOM | 4236 | CB | VAL | 751 | 59.129 | -4.724 | 30.485 | 1.00 | 33.81 |
| ATOM | 4237 | CG1 | VAL | 751 | 60.092 | -5.836 | 30.120 | 1.00 | 32.04 |
| ATOM | 4238 | CG2 | VAL | 751 | 59.415 | -3.535 | 29.598 | 1.00 | 30.67 |
| ATOM | 4239 | C | VAL | 751 | 57.428 | -6.493 | 31.131 | 1.00 | 41.68 |
| ATOM | 4240 | O | VAL | 751 | 57.492 | -7.599 | 30.594 | 1.00 | 39.92 |
| ATOM | 4241 | N | GLU | 752 | 57.109 | -6.338 | 32.414 | 1.00 | 44.22 |
| ATOM | 4242 | CA | GLU | 752 | 56.854 | -7.501 | 33.266 | 1.00 | 47.43 |
| ATOM | 4243 | CB | GLU | 752 | 56.779 | -7.078 | 34.743 | 1.00 | 49.29 |
| ATOM | 4244 | CG | GLU | 752 | 58.093 | -6.448 | 35.212 | 1.00 | 53.53 |
| ATOM | 4245 | CD | GLU | 752 | 58.215 | -6.249 | 36.707 | 1.00 | 53.05 |
| ATOM | 4246 | OE1 | GLU | 752 | 58.554 | -5.123 | 37.136 | 1.00 | 53.63 |
| ATOM | 4247 | OE2 | GLU | 752 | 58.021 | -7.228 | 37.452 | 1.00 | 56.18 |
| ATOM | 4248 | C | GLU | 752 | 55.594 | -8.256 | 32.809 | 1.00 | 46.90 |
| ATOM | 4249 | O | GLU | 752 | 55.646 | -9.464 | 32.551 | 1.00 | 43.85 |
| ATOM | 4250 | N | ASP | 753 | 54.490 | -7.529 | 32.640 | 1.00 | 48.05 |
| ATOM | 4251 | CA | ASP | 753 | 53.232 | -8.128 | 32.193 | 1.00 | 48.46 |
| ATOM | 4252 | CB | ASP | 753 | 52.119 | -7.090 | 32.118 | 1.00 | 51.25 |
| ATOM | 4253 | CG | ASP | 753 | 51.579 | -6.707 | 33.467 | 1.00 | 54.20 |
| ATOM | 4254 | OD1 | ASP | 753 | 51.440 | -7.589 | 34.330 | 1.00 | 57.31 |
| ATOM | 4255 | OD2 | ASP | 753 | 51.281 | -5.513 | 33.659 | 1.00 | 55.58 |
| ATOM | 4256 | C | ASP | 753 | 53.371 | -8.771 | 30.837 | 1.00 | 48.59 |
| ATOM | 4257 | O | ASP | 753 | 53.001 | -9.930 | 30.649 | 1.00 | 49.69 |
| ATOM | 4258 | N | LEU | 754 | 53.903 | -8.009 | 29.889 | 1.00 | 47.21 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4259 | CA | LEU | 754 | 54.102 | -8.489 | 28.523 | 1.00 | 46.37 |
| ATOM | 4260 | CB | LEU | 754 | 54.664 | -7.385 | 27.625 | 1.00 | 44.16 |
| ATOM | 4261 | CG | LEU | 754 | 53.621 | -6.366 | 27.152 | 1.00 | 46.35 |
| ATOM | 4262 | CD1 | LEU | 754 | 54.296 | -5.272 | 26.343 | 1.00 | 45.11 |
| ATOM | 4263 | CD2 | LEU | 754 | 52.514 | -7.070 | 26.349 | 1.00 | 42.89 |
| ATOM | 4264 | C | LEU | 754 | 55.004 | -9.703 | 28.481 | 1.00 | 47.08 |
| ATOM | 4265 | O | LEU | 754 | 54.818 | -10.590 | 27.659 | 1.00 | 45.02 |
| ATOM | 4266 | N | ASP | 755 | 55.969 | -9.755 | 29.385 | 1.00 | 49.68 |
| ATOM | 4267 | CA | ASP | 755 | 56.890 | -10.876 | 29.487 | 1.00 | 51.62 |
| ATOM | 4268 | CB | ASP | 755 | 57.883 | -10.586 | 30.615 | 1.00 | 54.90 |
| ATOM | 4269 | CG | ASP | 755 | 59.009 | -11.589 | 30.702 | 1.00 | 59.00 |
| ATOM | 4270 | OD1 | ASP | 755 | 59.694 | -11.608 | 31.746 | 1.00 | 63.70 |
| ATOM | 4271 | OD2 | ASP | 755 | 59.223 | -12.346 | 29.728 | 1.00 | 60.31 |
| ATOM | 4272 | C | ASP | 755 | 56.059 | -12.117 | 29.817 | 1.00 | 51.50 |
| ATOM | 4273 | O | ASP | 755 | 56.119 | -13.150 | 29.138 | 1.00 | 47.11 |
| ATOM | 4274 | N | ARG | 756 | 55.237 | -11.958 | 30.844 | 1.00 | 51.81 |
| ATOM | 4275 | CA | ARG | 756 | 54.362 | -13.009 | 31.328 | 1.00 | 51.44 |
| ATOM | 4276 | CB | ARG | 756 | 53.635 | -12.519 | 32.582 | 1.00 | 54.52 |
| ATOM | 4277 | CG | ARG | 756 | 52.459 | -13.358 | 33.027 | 1.00 | 55.00 |
| ATOM | 4278 | CD | ARG | 756 | 51.815 | -12.727 | 34.255 | 1.00 | 59.54 |
| ATOM | 4279 | NE | ARG | 756 | 51.417 | -11.335 | 34.026 | 1.00 | 64.01 |
| ATOM | 4280 | CZ | ARG | 756 | 50.366 | -10.960 | 33.301 | 1.00 | 65.76 |
| ATOM | 4281 | NH1 | ARG | 756 | 49.598 | -11.866 | 32.721 | 1.00 | 63.56 |
| ATOM | 4282 | NH2 | ARG | 756 | 50.061 | -9.676 | 33.183 | 1.00 | 66.59 |
| ATOM | 4283 | C | ARG | 756 | 53.361 | -13.440 | 30.260 | 1.00 | 50.03 |
| ATOM | 4284 | O | ARG | 756 | 53.267 | -14.622 | 29.960 | 1.00 | 49.98 |
| ATOM | 4285 | N | ILE | 757 | 52.645 | -12.483 | 29.673 | 1.00 | 46.87 |
| ATOM | 4286 | CA | ILE | 757 | 51.656 | -12.789 | 28.644 | 1.00 | 44.28 |
| ATOM | 4287 | CB | ILE | 757 | 50.919 | -11.532 | 28.125 | 1.00 | 40.46 |
| ATOM | 4288 | CG2 | ILE | 757 | 49.923 | -11.923 | 27.062 | 1.00 | 38.44 |
| ATOM | 4289 | CG1 | ILE | 757 | 50.202 | -10.830 | 29.277 | 1.00 | 39.74 |
| ATOM | 4290 | CD1 | ILE | 757 | 49.481 | -9.551 | 28.920 | 1.00 | 40.68 |
| ATOM | 4291 | C | ILE | 757 | 52.251 | -13.528 | 27.454 | 1.00 | 44.20 |
| ATOM | 4292 | O | ILE | 757 | 51.643 | -14.469 | 26.959 | 1.00 | 40.28 |
| ATOM | 4293 | N | VAL | 758 | 53.440 | -13.111 | 27.014 | 1.00 | 47.56 |
| ATOM | 4294 | CA | VAL | 758 | 54.102 | -13.745 | 25.874 | 1.00 | 48.90 |
| ATOM | 4295 | CB | VAL | 758 | 55.543 | -13.177 | 25.609 | 1.00 | 47.01 |
| ATOM | 4296 | CG1 | VAL | 758 | 56.198 | -13.920 | 24.456 | 1.00 | 44.38 |
| ATOM | 4297 | CG2 | VAL | 758 | 55.493 | -11.714 | 25.262 | 1.00 | 47.85 |
| ATOM | 4298 | C | VAL | 758 | 54.249 | -15.232 | 26.149 | 1.00 | 51.79 |
| ATOM | 4299 | O | VAL | 758 | 54.043 | -16.055 | 25.258 | 1.00 | 49.80 |
| ATOM | 4300 | N | ALA | 759 | 54.622 | -15.550 | 27.386 | 1.00 | 54.80 |
| ATOM | 4301 | CA | ALA | 759 | 54.825 | -16.925 | 27.814 | 1.00 | 57.15 |
| ATOM | 4302 | CB | ALA | 759 | 55.406 | -16.948 | 29.212 | 1.00 | 56.77 |
| ATOM | 4303 | C | ALA | 759 | 53.524 | -17.717 | 27.777 | 1.00 | 60.83 |
| ATOM | 4304 | O | ALA | 759 | 53.487 | -18.849 | 27.296 | 1.00 | 63.59 |
| ATOM | 4305 | N | LEU | 760 | 52.452 | -17.112 | 28.271 | 1.00 | 61.74 |
| ATOM | 4306 | CA | LEU | 760 | 51.151 | -17.760 | 28.295 | 1.00 | 61.29 |
| ATOM | 4307 | CB | LEU | 760 | 50.280 | -17.149 | 29.388 | 1.00 | 60.41 |
| ATOM | 4308 | CG | LEU | 760 | 50.808 | -17.323 | 30.812 | 1.00 | 58.68 |
| ATOM | 4309 | CD1 | LEU | 760 | 49.917 | -16.603 | 31.815 | 1.00 | 59.64 |
| ATOM | 4310 | CD2 | LEU | 760 | 50.899 | -18.799 | 31.138 | 1.00 | 57.84 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4311 | C | LEU | 760 | 50.439 | -17.706 | 26.951 | 1.00 | 63.42 |
| ATOM | 4312 | O | LEU | 760 | 49.282 | -18.121 | 26.842 | 1.00 | 63.68 |
| ATOM | 4313 | N | THR | 761 | 51.113 | -17.200 | 25.924 | 1.00 | 66.71 |
| ATOM | 4314 | CA | THR | 761 | 50.512 | -17.109 | 24.586 | 1.00 | 68.48 |
| ATOM | 4315 | CB | THR | 761 | 50.794 | -15.734 | 23.922 | 1.00 | 68.21 |
| ATOM | 4316 | OG1 | THR | 761 | 50.193 | -14.695 | 24.701 | 1.00 | 70.34 |
| ATOM | 4317 | CG2 | THR | 761 | 50.202 | -15.684 | 22.530 | 1.00 | 64.45 |
| ATOM | 4318 | C | THR | 761 | 51.030 | -18.225 | 23.688 | 1.00 | 69.65 |
| ATOM | 4319 | O | THR | 761 | 52.230 | -18.492 | 23.623 | 1.00 | 70.43 |
| ATOM | 4320 | SG | CYS | 1603 | 18.668 | -9.074 | 20.131 | 0.50 | 30.57 |
| ATOM | 4321 | CG | MET | 534 | 69.414 | 12.079 | 23.224 | 0.50 | 36.86 |
| ATOM | 4322 | SD | MET | 534 | 69.162 | 13.149 | 24.646 | 0.50 | 40.20 |
| ATOM | 4323 | CE | MET | 534 | 70.204 | 12.299 | 25.912 | 0.50 | 41.95 |
| ATOM | 4324 | SG | CYS | 603 | 56.218 | -8.072 | 16.341 | 0.50 | 37.35 |
| ATOM | 4325 | OH2 | TIP | 1 | 71.863 | 25.340 | 2.719 | 1.00 | 24.40 |
| ATOM | 4326 | OH2 | TIP | 2 | 39.671 | 4.177 | 15.837 | 1.00 | 36.87 |
| ATOM | 4327 | OH2 | TIP | 3 | 83.765 | 19.802 | 10.549 | 1.00 | 26.81 |
| ATOM | 4328 | OH2 | TIP | 4 | 83.844 | 20.193 | 7.757 | 1.00 | 30.07 |
| ATOM | 4329 | OH2 | TIP | 5 | 75.192 | 16.430 | 6.693 | 1.00 | 26.76 |
| ATOM | 4330 | OH2 | TIP | 6 | 86.579 | 19.662 | 9.323 | 1.00 | 36.11 |
| ATOM | 4331 | OH2 | TIP | 7 | 52.204 | 10.911 | 24.392 | 1.00 | 36.83 |
| ATOM | 4332 | OH2 | TIP | 8 | 55.174 | 9.435 | 22.514 | 1.00 | 21.93 |
| ATOM | 4333 | OH2 | TIP | 9 | 57.077 | 4.556 | 32.580 | 1.00 | 25.17 |
| ATOM | 4334 | OH2 | TIP | 10 | 52.281 | 4.737 | 13.300 | 1.00 | 20.79 |
| ATOM | 4335 | OH2 | TIP | 11 | 41.402 | 5.304 | 22.893 | 1.00 | 39.17 |
| ATOM | 4336 | OH2 | TIP | 12 | 45.088 | 8.857 | 21.604 | 1.00 | 35.14 |
| ATOM | 4337 | OH2 | TIP | 13 | 64.519 | -2.772 | 28.799 | 1.00 | 47.52 |
| ATOM | 4338 | OH2 | TIP | 14 | 77.327 | 12.960 | 23.832 | 1.00 | 34.47 |
| ATOM | 4339 | OH2 | TIP | 15 | 79.366 | 17.021 | 18.247 | 1.00 | 47.49 |
| ATOM | 4340 | OH2 | TIP | 16 | 83.087 | 11.573 | 15.986 | 1.00 | 22.80 |
| ATOM | 4341 | OH2 | TIP | 17 | 13.977 | -9.804 | 0.222 | 1.00 | 24.88 |
| ATOM | 4342 | OH2 | TIP | 18 | 38.451 | 0.155 | 5.081 | 1.00 | 41.03 |
| ATOM | 4343 | OH2 | TIP | 20 | 27.109 | 6.286 | 4.902 | 1.00 | 27.69 |
| ATOM | 4344 | OH2 | TIP | 21 | 34.379 | -1.750 | 16.771 | 1.00 | 47.69 |
| ATOM | 4345 | OH2 | TIP | 22 | 20.394 | 2.449 | 27.821 | 1.00 | 54.32 |
| ATOM | 4346 | OH2 | TIP | 23 | 50.587 | -11.642 | 38.062 | 1.00 | 45.31 |
| ATOM | 4347 | OH2 | TIP | 24 | 17.137 | -5.949 | -1.716 | 1.00 | 27.63 |
| ATOM | 4348 | OH2 | TIP | 25 | 27.604 | 7.961 | 15.119 | 1.00 | 47.19 |
| ATOM | 4349 | OH2 | TIP | 26 | 31.446 | 0.136 | 6.605 | 1.00 | 29.98 |
| ATOM | 4350 | OH2 | TIP | 27 | 27.030 | -13.047 | 27.803 | 1.00 | 28.86 |
| ATOM | 4351 | OH2 | TIP | 28 | 28.477 | -17.191 | 13.067 | 1.00 | 37.44 |
| ATOM | 4352 | OH2 | TIP | 29 | 88.748 | 14.279 | 8.091 | 1.00 | 32.72 |
| ATOM | 4353 | OH2 | TIP | 30 | -2.392 | -3.684 | 11.343 | 1.00 | 41.86 |
| ATOM | 4354 | OH2 | TIP | 31 | 34.968 | -4.221 | 18.549 | 1.00 | 40.51 |
| ATOM | 4355 | OH2 | TIP | 32 | 80.581 | 17.982 | 9.655 | 1.00 | 27.85 |
| ATOM | 4356 | OH2 | TIP | 33 | 5.522 | 3.773 | 10.805 | 1.00 | 24.60 |
| ATOM | 4357 | OH2 | TIP | 34 | -10.747 | 5.416 | 11.174 | 1.00 | 29.27 |
| ATOM | 4358 | OH2 | TIP | 35 | 29.049 | -8.816 | 19.978 | 1.00 | 35.24 |
| ATOM | 4359 | OH2 | TIP | 36 | 5.871 | 3.463 | 13.481 | 1.00 | 26.62 |
| ATOM | 4360 | OH2 | TIP | 37 | 31.834 | 2.899 | 0.207 | 1.00 | 49.70 |
| ATOM | 4361 | OH2 | TIP | 38 | 19.799 | 2.012 | -3.941 | 1.00 | 29.67 |
| ATOM | 4362 | OH2 | TIP | 39 | 62.060 | 2.679 | 32.659 | 1.00 | 54.86 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4363 | OH2 | TIP | 40 | 21.100 | -6.883 | -4.054 | 1.00 | 22.33 |
| ATOM | 4364 | OH2 | TIP | 41 | -15.675 | 8.744 | 22.559 | 1.00 | 44.54 |
| ATOM | 4365 | OH2 | TIP | 42 | 40.066 | 2.225 | 8.567 | 1.00 | 57.00 |
| ATOM | 4366 | OH2 | TIP | 43 | 19.477 | 11.293 | -0.049 | 1.00 | 37.77 |
| ATOM | 4367 | OH2 | TIP | 44 | 67.060 | 9.047 | 17.334 | 1.00 | 25.14 |
| ATOM | 4368 | OH2 | TIP | 45 | 87.829 | 18.937 | 18.529 | 1.00 | 45.92 |
| ATOM | 4369 | OH2 | TIP | 46 | 74.741 | 16.956 | 3.987 | 1.00 | 40.33 |
| ATOM | 4370 | OH2 | TIP | 47 | 29.411 | 16.888 | 10.525 | 1.00 | 38.41 |
| ATOM | 4371 | OH2 | TIP | 48 | 66.592 | 7.020 | 15.108 | 1.00 | 36.15 |
| ATOM | 4372 | OH2 | TIP | 49 | 85.071 | 21.432 | 5.755 | 1.00 | 19.89 |
| ATOM | 4373 | OH2 | TIP | 50 | -4.842 | 3.281 | 3.118 | 1.00 | 28.22 |
| ATOM | 4374 | OH2 | TIP | 51 | 19.454 | 5.250 | 4.876 | 1.00 | 34.86 |
| ATOM | 4375 | OH2 | TIP | 53 | 34.785 | 5.433 | 24.743 | 1.00 | 30.40 |
| ATOM | 4376 | OH2 | TIP | 54 | 34.792 | -17.150 | 13.665 | 1.00 | 35.81 |
| ATOM | 4377 | OH2 | TIP | 55 | 59.956 | 7.380 | 27.941 | 1.00 | 36.76 |
| ATOM | 4378 | OH2 | TIP | 56 | -7.327 | -1.518 | 6.428 | 1.00 | 39.13 |
| ATOM | 4379 | OH2 | TIP | 57 | 55.164 | 12.120 | 25.338 | 1.00 | 38.87 |
| ATOM | 4380 | OH2 | TIP | 58 | 68.637 | 6.832 | 16.698 | 1.00 | 54.96 |
| ATOM | 4381 | OH2 | TIP | 59 | 73.778 | 20.869 | 19.031 | 1.00 | 35.01 |
| ATOM | 4382 | OH2 | TIP | 60 | 3.582 | -8.363 | -8.103 | 1.00 | 16.71 |
| ATOM | 4383 | OH2 | TIP | 61 | 38.051 | 10.933 | 5.487 | 1.00 | 32.85 |
| ATOM | 4384 | OH2 | TIP | 62 | 29.727 | -9.630 | -1.370 | 1.00 | 30.92 |
| ATOM | 4385 | OH2 | TIP | 64 | 49.186 | 1.253 | 12.066 | 1.00 | 42.67 |
| ATOM | 4386 | OH2 | TIP | 65 | 41.375 | 3.989 | 28.951 | 1.00 | 37.95 |
| ATOM | 4387 | OH2 | TIP | 66 | 10.798 | -13.119 | 1.125 | 1.00 | 38.26 |
| ATOM | 4388 | OH2 | TIP | 67 | -1.079 | -4.386 | 21.428 | 1.00 | 27.92 |
| ATOM | 4389 | OH2 | TIP | 68 | 30.327 | 16.346 | 13.295 | 1.00 | 53.21 |
| ATOM | 4390 | OH2 | TIP | 69 | 8.319 | 4.437 | 3.449 | 1.00 | 23.63 |
| ATOM | 4391 | OH2 | TIP | 70 | 73.152 | 18.809 | 22.631 | 1.00 | 36.45 |
| ATOM | 4392 | OH2 | TIP | 71 | -7.984 | -3.476 | 25.048 | 1.00 | 33.16 |
| ATOM | 4393 | OH2 | TIP | 72 | 66.529 | -4.720 | 28.421 | 1.00 | 66.32 |
| ATOM | 4394 | OH2 | TIP | 73 | 21.577 | -20.723 | 4.868 | 1.00 | 48.14 |
| ATOM | 4395 | OH2 | TIP | 74 | 59.417 | -6.760 | 4.957 | 1.00 | 48.73 |
| ATOM | 4396 | OH2 | TIP | 75 | 16.509 | -13.306 | -2.942 | 1.00 | 41.02 |
| ATOM | 4397 | OH2 | TIP | 76 | -15.064 | 7.473 | 4.275 | 1.00 | 26.77 |
| ATOM | 4398 | OH2 | TIP | 77 | 33.118 | 2.917 | 13.384 | 1.00 | 41.38 |
| ATOM | 4399 | OH2 | TIP | 78 | 0.112 | -2.913 | 10.809 | 1.00 | 27.49 |
| ATOM | 4400 | OH2 | TIP | 79 | 17.448 | 2.562 | 5.507 | 1.00 | 16.32 |
| ATOM | 4401 | OH2 | TIP | 81 | 27.445 | 3.796 | 6.134 | 1.00 | 29.83 |
| ATOM | 4402 | OH2 | TIP | 82 | -8.708 | 6.231 | 9.598 | 1.00 | 27.66 |
| ATOM | 4403 | OH2 | TIP | 83 | 1.565 | -1.998 | 8.758 | 1.00 | 33.46 |
| ATOM | 4404 | OH2 | TIP | 84 | -4.774 | -3.153 | 7.049 | 1.00 | 36.59 |
| ATOM | 4405 | OH2 | TIP | 85 | 17.443 | 3.105 | 1.795 | 1.00 | 20.39 |
| ATOM | 4406 | OH2 | TIP | 86 | 20.120 | 3.387 | 2.918 | 1.00 | 30.35 |
| ATOM | 4407 | OH2 | TIP | 87 | 0.466 | -2.238 | 22.190 | 1.00 | 20.30 |
| ATOM | 4408 | OH2 | TIP | 88 | 19.749 | -6.018 | -1.687 | 1.00 | 21.33 |
| ATOM | 4409 | OH2 | TIP | 89 | 10.505 | -15.695 | 6.861 | 1.00 | 38.80 |
| ATOM | 4410 | OH2 | TIP | 90 | 4.223 | -12.113 | 11.774 | 1.00 | 34.18 |
| ATOM | 4411 | OH2 | TIP | 91 | 6.297 | 1.090 | -3.192 | 1.00 | 24.40 |
| ATOM | 4412 | OH2 | TIP | 92 | -13.540 | 1.554 | 5.413 | 1.00 | 34.94 |
| ATOM | 4413 | OH2 | TIP | 93 | 15.607 | -7.315 | 0.017 | 1.00 | 26.30 |
| ATOM | 4414 | OH2 | TIP | 94 | -1.868 | -5.461 | 3.839 | 1.00 | 37.12 |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4415 | OH2 | TIP | 95 | 12.718 | 5.095 | -4.401 | 1.00 | 40.61 |
| ATOM | 4416 | OH2 | TIP | 96 | 69.849 | 27.233 | 2.056 | 1.00 | 41.42 |
| ATOM | 4417 | OH2 | TIP | 97 | 24.374 | -13.311 | 0.143 | 1.00 | 52.75 |
| ATOM | 4418 | OH2 | TIP | 98 | 60.424 | -4.582 | 34.237 | 1.00 | 42.02 |
| ATOM | 4419 | OH2 | TIP | 99 | 10.589 | 5.757 | 3.485 | 1.00 | 61.53 |
| ATOM | 4420 | OH2 | TIP | 100 | -9.564 | -3.999 | 4.718 | 1.00 | 29.02 |
| ATOM | 4421 | OH2 | TIP | 101 | 73.085 | -1.967 | 10.565 | 1.00 | 59.23 |
| ATOM | 4422 | OH2 | TIP | 102 | -3.172 | 5.701 | 30.623 | 1.00 | 30.51 |
| ATOM | 4423 | OH2 | TIP | 103 | 36.672 | 0.620 | 11.780 | 1.00 | 53.77 |
| ATOM | 4424 | OH2 | TIP | 104 | 21.408 | 6.462 | 16.955 | 1.00 | 27.62 |
| ATOM | 4425 | OH2 | TIP | 105 | 31.224 | 0.791 | 19.345 | 1.00 | 77.65 |
| ATOM | 4426 | OH2 | TIP | 106 | 5.660 | -8.451 | 22.197 | 1.00 | 49.50 |
| ATOM | 4427 | OH2 | TIP | 107 | -12.988 | 8.471 | 17.441 | 1.00 | 31.69 |
| ATOM | 4428 | OH2 | TIP | 108 | 26.733 | -10.524 | -0.894 | 1.00 | 25.26 |
| ATOM | 4429 | OH2 | TIP | 109 | 24.182 | 2.026 | 18.156 | 1.00 | 35.87 |
| ATOM | 4430 | OH2 | TIP | 110 | -1.822 | 12.848 | 3.561 | 1.00 | 35.44 |
| ATOM | 4431 | OH2 | TIP | 111 | 59.584 | 13.491 | 33.225 | 1.00 | 40.47 |
| ATOM | 4432 | OH2 | TIP | 112 | 4.402 | -10.813 | 1.929 | 1.00 | 47.07 |
| ATOM | 4433 | OH2 | TIP | 113 | 8.032 | 2.916 | 0.940 | 1.00 | 40.79 |
| ATOM | 4434 | OH2 | TIP | 114 | 75.905 | 1.522 | 25.912 | 1.00 | 55.51 |
| ATOM | 4435 | OH2 | TIP | 115 | 48.960 | 15.737 | 14.249 | 1.00 | 38.97 |
| ATOM | 4436 | OH2 | TIP | 116 | 2.333 | -11.271 | 9.174 | 1.00 | 29.12 |
| ATOM | 4437 | OH2 | TIP | 117 | 83.062 | 26.404 | 12.925 | 1.00 | 41.17 |
| ATOM | 4438 | OH2 | TIP | 118 | 8.816 | -6.440 | -3.424 | 1.00 | 48.26 |
| ATOM | 4439 | OH2 | TIP | 119 | -8.594 | 4.575 | 4.258 | 1.00 | 32.68 |
| ATOM | 4440 | OH2 | TIP | 120 | 7.695 | -13.769 | 8.481 | 1.00 | 39.22 |
| ATOM | 4441 | OH2 | TIP | 121 | 51.500 | 6.285 | 10.369 | 1.00 | 25.18 |
| ATOM | 4442 | OH2 | TIP | 122 | 20.720 | 3.849 | 15.625 | 1.00 | 22.46 |
| ATOM | 4443 | OH2 | TIP | 123 | 73.111 | 3.718 | 20.617 | 1.00 | 28.26 |
| ATOM | 4444 | OH2 | TIP | 124 | 5.312 | -11.608 | 22.516 | 1.00 | 32.74 |
| ATOM | 4445 | OH2 | TIP | 125 | 34.207 | 2.437 | 16.601 | 1.00 | 65.04 |
| ATOM | 4446 | OH2 | TIP | 126 | 9.535 | -11.998 | 7.085 | 1.00 | 25.13 |
| ATOM | 4447 | OH2 | TIP | 127 | 8.227 | 3.912 | -1.495 | 1.00 | 43.73 |
| ATOM | 4448 | OH2 | TIP | 129 | 7.312 | 7.072 | 2.922 | 1.00 | 47.65 |
| ATOM | 4449 | OH2 | TIP | 130 | 35.824 | -1.660 | 0.135 | 1.00 | 30.43 |
| ATOM | 4450 | OH2 | TIP | 131 | 44.723 | 10.285 | 11.144 | 1.00 | 32.74 |
| ATOM | 4451 | OH2 | TIP | 132 | 27.941 | -13.172 | 18.733 | 1.00 | 58.65 |
| ATOM | 4452 | OH2 | TIP | 133 | 45.301 | 11.497 | 21.408 | 1.00 | 35.00 |
| ATOM | 4453 | OH2 | TIP | 134 | 57.705 | -10.824 | 14.202 | 1.00 | 69.18 |
| ATOM | 4454 | OH2 | TIP | 135 | -3.108 | 15.385 | 16.685 | 1.00 | 38.07 |
| ATOM | 4455 | OH2 | TIP | 136 | 85.884 | 11.182 | 9.044 | 1.00 | 32.04 |
| ATOM | 4456 | OH2 | TIP | 137 | 12.840 | -2.444 | 1.983 | 1.00 | 30.08 |
| ATOM | 4457 | OH2 | TIP | 138 | 75.645 | 3.496 | 20.607 | 1.00 | 33.94 |
| ATOM | 4458 | OH2 | TIP | 139 | 13.020 | 7.518 | -2.510 | 1.00 | 40.68 |
| ATOM | 4459 | OH2 | TIP | 140 | 11.245 | -10.070 | 0.729 | 1.00 | 26.02 |
| ATOM | 4460 | OH2 | TIP | 141 | 59.563 | 10.829 | 14.466 | 1.00 | 71.34 |
| ATOM | 4461 | OH2 | TIP | 142 | 13.671 | -16.214 | 3.489 | 1.00 | 39.47 |
| ATOM | 4462 | OH2 | TIP | 143 | -6.358 | -3.421 | 16.520 | 1.00 | 37.08 |
| ATOM | 4463 | OH2 | TIP | 144 | 25.629 | -12.764 | 3.534 | 1.00 | 50.51 |
| ATOM | 4464 | OH2 | TIP | 145 | -16.459 | 10.869 | 6.524 | 1.00 | 38.40 |
| ATOM | 4465 | OH2 | TIP | 146 | 86.598 | 12.840 | 7.028 | 1.00 | 47.80 |
| ATOM | 4466 | OH2 | TIP | 147 | 32.139 | -4.674 | 1.757 | 1.00 | 32.43 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4467 | OH2 | TIP | 148 | 44.890 | 7.505 | 11.806 | 1.00 | 32.46 |
| ATOM | 4468 | OH2 | TIP | 149 | 80.781 | 12.432 | 16.562 | 1.00 | 47.77 |
| ATOM | 4469 | OH2 | TIP | 150 | 3.017 | -7.101 | -1.917 | 1.00 | 40.92 |
| ATOM | 4470 | OH2 | TIP | 151 | 31.784 | -6.139 | 20.968 | 1.00 | 38.23 |
| ATOM | 4471 | OH2 | TIP | 152 | 74.835 | -2.597 | 12.290 | 1.00 | 48.89 |
| ATOM | 4472 | OH2 | TIP | 153 | 7.509 | 6.768 | -1.083 | 1.00 | 46.02 |
| ATOM | 4473 | OH2 | TIP | 154 | 71.732 | 5.360 | 21.908 | 1.00 | 33.30 |
| ATOM | 4474 | OH2 | TIP | 155 | 68.150 | -5.075 | 8.794 | 1.00 | 39.31 |
| ATOM | 4475 | OH2 | TIP | 156 | 0.148 | -9.544 | 6.872 | 1.00 | 41.37 |
| ATOM | 4476 | OH2 | TIP | 157 | 67.878 | 18.204 | 10.861 | 1.00 | 51.19 |
| ATOM | 4477 | OH2 | TIP | 158 | 3.652 | 8.829 | 4.428 | 1.00 | 31.24 |
| ATOM | 4478 | OH2 | TIP | 159 | 52.100 | 11.362 | 18.433 | 1.00 | 40.73 |
| ATOM | 4479 | OH2 | TIP | 161 | -10.357 | 6.783 | 4.861 | 1.00 | 35.13 |
| ATOM | 4480 | OH2 | TIP | 162 | 76.471 | 1.562 | -0.853 | 1.00 | 59.17 |
| ATOM | 4481 | OH2 | TIP | 163 | 10.073 | -12.056 | 17.071 | 1.00 | 44.69 |
| ATOM | 4482 | OH2 | TIP | 164 | 34.163 | 14.271 | 18.254 | 1.00 | 39.59 |
| ATOM | 4483 | OH2 | TIP | 165 | 2.320 | -7.990 | 16.820 | 1.00 | 38.19 |
| ATOM | 4484 | OH2 | TIP | 166 | 29.696 | 1.908 | 6.098 | 1.00 | 38.02 |
| ATOM | 4485 | OH2 | TIP | 167 | 32.626 | -17.410 | 11.766 | 1.00 | 48.15 |
| ATOM | 4486 | OH2 | TIP | 168 | 42.244 | 18.049 | 11.043 | 1.00 | 50.95 |
| ATOM | 4487 | OH2 | TIP | 169 | 87.907 | 10.574 | 5.721 | 1.00 | 60.28 |
| ATOM | 4488 | OH2 | TIP | 170 | 70.313 | -3.998 | 25.141 | 1.00 | 72.64 |
| ATOM | 4489 | OH2 | TIP | 171 | 77.603 | 5.679 | 23.952 | 1.00 | 43.23 |
| ATOM | 4490 | OH2 | TIP | 172 | -0.942 | -8.153 | 4.508 | 1.00 | 55.10 |
| ATOM | 4491 | OH2 | TIP | 173 | 34.297 | 15.574 | 1.690 | 1.00 | 34.19 |
| ATOM | 4492 | OH2 | TIP | 174 | -9.643 | 7.829 | 7.414 | 1.00 | 50.48 |
| ATOM | 4493 | OH2 | TIP | 175 | 11.618 | 5.655 | 7.455 | 1.00 | 43.37 |
| ATOM | 4494 | OH2 | TIP | 176 | -8.705 | 13.841 | 13.642 | 1.00 | 72.49 |
| ATOM | 4495 | OH2 | TIP | 177 | 32.009 | 3.416 | 18.257 | 1.00 | 44.16 |
| ATOM | 4496 | OH2 | TIP | 178 | -8.651 | 10.180 | 24.352 | 1.00 | 44.85 |
| ATOM | 4497 | OH2 | TIP | 179 | -1.153 | -6.532 | 15.548 | 1.00 | 32.90 |
| ATOM | 4498 | OH2 | TIP | 180 | 80.235 | 0.749 | 15.508 | 1.00 | 34.75 |
| ATOM | 4499 | OH2 | TIP | 181 | 67.222 | 20.490 | -1.574 | 1.00 | 40.76 |
| ATOM | 4500 | OH2 | TIP | 182 | -0.471 | 4.367 | 1.248 | 1.00 | 36.58 |
| ATOM | 4501 | OH2 | TIP | 183 | 0.149 | 6.517 | 2.578 | 1.00 | 40.12 |
| ATOM | 4502 | OH2 | TIP | 184 | -1.186 | 8.867 | 1.311 | 1.00 | 44.77 |
| ATOM | 4503 | OH2 | TIP | 185 | -5.093 | 9.260 | 2.252 | 1.00 | 52.07 |
| ATOM | 4504 | OH2 | TIP | 186 | -7.235 | 10.227 | 3.913 | 1.00 | 58.53 |
| ATOM | 4505 | OH2 | TIP | 187 | 2.724 | 7.169 | 0.879 | 1.00 | 47.77 |
| ATOM | 4506 | OH2 | TIP | 188 | 5.527 | 11.031 | 8.519 | 1.00 | 34.40 |
| ATOM | 4507 | OH2 | TIP | 189 | 63.927 | 12.721 | 22.689 | 1.00 | 40.75 |
| ATOM | 4508 | OH2 | TIP | 190 | 79.264 | 1.066 | 18.321 | 1.00 | 41.34 |
| ATOM | 4509 | OH2 | TIP | 191 | 59.247 | -11.825 | 7.256 | 1.00 | 79.86 |
| ATOM | 4510 | OH2 | TIP | 192 | 13.994 | -0.972 | -4.310 | 1.00 | 31.15 |
| ATOM | 4511 | OH2 | TIP | 193 | 59.546 | 3.024 | 33.227 | 1.00 | 40.34 |
| ATOM | 4512 | OH2 | TIP | 194 | 32.179 | 13.637 | 19.964 | 1.00 | 48.25 |
| ATOM | 4513 | OH2 | TIP | 195 | 72.178 | 16.188 | 22.879 | 1.00 | 42.72 |
| ATOM | 4514 | OH2 | TIP | 196 | 0.898 | -8.663 | 14.348 | 1.00 | 41.76 |
| ATOM | 4515 | OH2 | TIP | 197 | -0.490 | 5.455 | 30.574 | 1.00 | 38.30 |
| ATOM | 4516 | OH2 | TIP | 199 | -1.277 | -4.244 | 27.691 | 1.00 | 56.27 |
| ATOM | 4517 | OH2 | TIP | 200 | 81.605 | 15.360 | 17.272 | 1.00 | 42.05 |
| ATOM | 4518 | OH2 | TIP | 201 | -17.534 | 4.081 | 23.779 | 1.00 | 59.65 |

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ATOM   4519  OH2 TIP   202      27.748  10.634  14.595  1.00 49.97
ATOM   4520  OH2 TIP   203      34.891   4.468  27.604  1.00 60.26
ATOM   4521  OH2 TIP   204      -3.460  -4.448   9.045  1.00 44.70
ATOM   4522  OH2 TIP   205      42.705   7.590  22.526  1.00 35.77
ATOM   4523  OH2 TIP   206      52.983  11.950  21.969  1.00 35.12
ATOM   4524  OH2 TIP   207      26.871  14.098  19.820  1.00 53.04
ATOM   4525  OH2 TIP   208      -7.184   9.323   6.370  1.00 37.49
ATOM   4526  OH2 TIP   209      86.676   5.553  15.911  1.00 72.92
ATOM   4527  OH2 TIP   210      55.080  15.928  20.414  1.00 68.75
ATOM   4528  OH2 TIP   211      51.512  19.264  22.672  1.00 54.72
ATOM   4529  OH2 TIP   212      19.988   7.127   6.976  1.00 45.55
ATOM   4530  OH2 TIP   213      28.905   2.021  -3.430  1.00 48.55
ATOM   4531  OH2 TIP   214      26.446   2.593  -4.753  1.00 55.04
ATOM   4532  OH2 TIP   215      36.539   2.911  18.446  1.00 38.50
ATOM   4533  OH2 TIP   216      16.807 -20.725  14.119  1.00 56.03
ATOM   4534  OH2 TIP   217      28.203 -14.485   6.172  1.00 62.90
ATOM   4535  OH2 TIP   218      31.519   1.503  -2.010  1.00 56.19
ATOM   4536  OH2 TIP   219      10.014 -16.571  15.451  1.00 46.37
ATOM   4537  OH2 TIP   220       7.126 -11.922   5.526  1.00 56.89
ATOM   4538  OH2 TIP   221     -12.414  14.643  10.965  1.00 67.36
ATOM   4539  OH2 TIP   222      10.978   9.734  -1.436  1.00 38.81
ATOM   4540  OH2 TIP   223      11.293  12.362  -1.306  1.00 52.56
ATOM   4541  OH2 TIP   224      34.011  13.162  -1.255  1.00 52.58
ATOM   4542  OH2 TIP   225      31.195  17.923   8.021  1.00 75.88
ATOM   4543  OH2 TIP   226      36.957  11.949  -1.947  1.00 50.99
ATOM   4544  OH2 TIP   227      35.179   3.114  10.888  1.00 58.55
ATOM   4545  OH2 TIP   228      64.027  13.281  26.577  1.00 51.98
ATOM   4546  OH2 TIP   229      36.514   6.155  15.292  1.00 45.57
ATOM   4547  OH2 TIP   230      90.627   4.339   6.386  1.00 56.65
ATOM   4548  OH2 TIP   231      49.907 -11.937  10.792  1.00 53.49
ATOM   4549  OH2 TIP   232      60.296 -10.212  16.610  1.00 79.85
ATOM   4550  OH2 TIP   233      18.154 -21.314   7.018  1.00 53.60
ATOM   4551  OH2 TIP   234      66.186  -1.068  30.882  1.00 56.92
ATOM   4552  OH2 TIP   235      75.153  18.983  20.700  1.00 34.22
ATOM   4553  OH2 TIP   236      -2.885  10.207   3.295  1.00 68.34
ATOM   4554  OH2 TIP   237       5.834  -3.507  25.370  1.00 34.75
ATOM   4555  OH2 TIP   238      35.910   6.163  12.569  1.00 37.31
ATOM   4556  OH2 TIP   239      -5.494  16.637  14.033  1.00 65.17
ATOM   4557  OH2 TIP   240      46.332 -11.698  26.865  1.00 55.30
ATOM   4558  OH2 TIP   241       6.179   6.434  13.895  1.00 45.92
ATOM   4559  OH2 TIP   242      -3.869  -4.958  20.821  1.00 41.96
ATOM   4560  OH2 TIP   243       1.690  -3.598  -0.200  1.00 41.42
ATOM   4561  OH2 TIP   244      86.181  11.454  23.000  1.00 56.22
ATOM   4562  OH2 TIP   245      10.501   7.621   5.627  1.00 77.40
ATOM   4563  OH2 TIP   246       5.007   8.485   2.181  1.00 89.31
ATOM   4564  OH2 TIP   247      64.552  -8.093  20.595  1.00 45.86
ATOM   4565  OH2 TIP   248      11.243 -17.828  13.332  1.00 65.30
ATOM   4566  OH2 TIP   249      42.226  -6.785  14.857  1.00 81.78
ATOM   4567  OH2 TIP   250       2.875  -4.176  22.032  1.00 53.45
ATOM   4568  OH2 TIP   251      72.048   1.134  -2.037  1.00 38.85
ATOM   4569  OH2 TIP   252      50.357  -3.142  32.887  1.00 67.13
ATOM   4570  OH2 TIP   254      57.772   9.500  11.808  1.00 40.03
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ATOM   4571  OH2 TIP   255       43.306  20.459  30.366  1.00 47.59
ATOM   4572  OH2 TIP   256       67.064  16.514  15.765  1.00 57.51
ATOM   4573  OH2 TIP   257       87.612  21.648   5.147  1.00 70.52
ATOM   4574  OH2 TIP   258       21.095   9.853  -9.308  1.00 78.97
ATOM   4575  OH2 TIP   261       71.914  28.544   7.912  1.00 83.90
ATOM   4576  OH2 TIP   262       25.727  -8.133  27.190  1.00 54.87
ATOM   4577  OH2 TIP   263      -18.738  10.877  12.767  1.00 71.80
ATOM   4578  OH2 TIP   264       30.524  11.543  16.329  1.00 46.98
ATOM   4579  OH2 TIP   265       22.211 -16.242  -2.763  1.00 55.17
ATOM   4580  OH2 TIP   266       29.755   9.037  18.396  1.00 67.93
ATOM   4581  C1  MON  1000       67.458   4.500  11.935  1.00  0.00
ATOM   4582  C2  MON  1000       67.015   3.958  10.687  1.00  0.00
ATOM   4583  N3  MON  1000       67.367   2.732  10.160  1.00  0.00
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ATOM   4586  C6  MON  1000       66.041   6.508  11.380  1.00  0.00
ATOM   4587  C7  MON  1000       66.948   5.809  12.276  1.00  0.00
ATOM   4588  C8  MON  1000       65.933   3.759   8.668  1.00  0.00
ATOM   4589  C10 MON  1000       66.745   2.518   8.922  1.00  0.00
ATOM   4590  C11 MON  1000       65.043   4.051   7.483  1.00  0.00
ATOM   4591  O12 MON  1000       66.862   1.516   8.241  1.00  0.00
ATOM   4592  C13 MON  1000       64.479   2.990   6.570  1.00  0.00
ATOM   4593  C14 MON  1000       63.459   3.330   5.617  1.00  0.00
ATOM   4594  C15 MON  1000       62.923   2.333   4.727  1.00  0.00
ATOM   4595  C16 MON  1000       63.379   0.956   4.754  1.00  0.00
ATOM   4596  C17 MON  1000       64.960   1.637   6.605  1.00  0.00
ATOM   4597  C18 MON  1000       64.418   0.642   5.713  1.00  0.00
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ATOM   4601  C22 MON  1000       61.085  -0.818   2.152  1.00  0.00
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ATOM   4603  C24 MON  1000       62.562  -2.492   3.133  1.00  0.00
ATOM   4604  O25 MON  1000       61.481  -2.328  -0.389  1.00  0.00
ATOM   4605  C26 MON  1000       62.001  -2.670   0.659  1.00  0.00
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ATOM   4620  C16 MON  1001       10.435   3.935  25.881  1.00  0.00
ATOM   4621  C17 MON  1001        8.670   3.508  24.123  1.00  0.00
ATOM   4622  C18 MON  1001        9.416   3.095  25.285  1.00  0.00
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ATOM    4623   N19  MON   1001       11.168    3.525   27.023   1.00   0.00
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ATOM    4625   C21  MON   1001       12.107    4.463   27.725   1.00   0.00
ATOM    4626   C22  MON   1001       13.125    3.821   28.698   1.00   0.00
ATOM    4627   N23  MON   1001       12.570    2.742   29.518   1.00   0.00
ATOM    4628   C24  MON   1001       11.902    1.711   28.725   1.00   0.00
ATOM    4629   O25  MON   1001       13.118    3.569   31.669   1.00   0.00
ATOM    4630   C26  MON   1001       12.610    2.731   30.944   1.00   0.00
```

## CLAIMS

What is claimed is:

1. A crystalline form of a polypeptide corresponding to the catalytic domain of a protein tyrosine kinase.

2. The crystalline form of claim 1, wherein said protein tyrosine kinase is a receptor protein tyrosine kinase.

3. The crystalline form of claim 2, wherein said receptor protein tyrosine kinase is selected from the group consisting of PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.

4. The crystalline form of claim 1, wherein said protein tyrosine kinase is a non-receptor protein tyrosine kinase.

5. The crystalline form of claim 4, wherein said non-receptor protein tyrosine kinase is selected from a group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

6. The crystalline form of claim 1, comprising one or more heavy metal atoms.

7. The crystalline form of claim 1, wherein said

protein tyrosine kinase is FGFR.

8. The crystalline form of claim 7, wherein said FGFR is FGFR1.

9. The crystalline form of claim 8, defined by atomic structural coordinates set forth in Table 1.

10. The crystalline form of claim 7, comprising at least one compound.

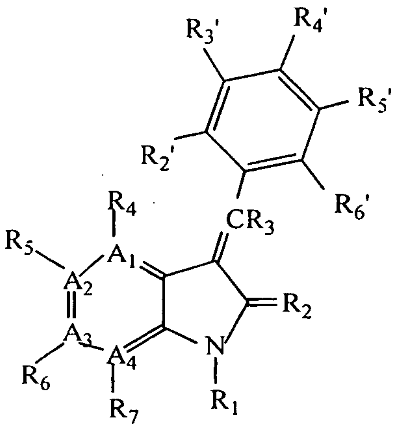
11. The crystalline form of claim 10, wherein said compound is a nucleotide analog.

12. The crystalline form of claim 11, wherein said nucleotide analog is AMP-PCP.

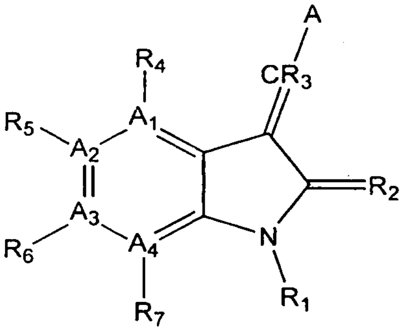
13. The crystalline form of claim 12, defined by atomic structural coordinates set forth in Table 2.

14. The crystalline form of claim 10, wherein said compound is an indolinone compound.

15. The crystalline form of claim 14, wherein said indolinone compound has a structure set forth in formula I or II:



(I)



(II)

or a pharmaceutically acceptable salt, isomer, metabolite, ester, amide, or prodrug thereof, wherein

(a) $A_1$, $A_2$, $A_3$, and $A_4$ are independently carbon or nitrogen;

(b) $R_1$ is hydrogen or alkyl;

(c) $R_2$ is oxygen in the case of an oxindolinone or sulfur in the case of a thiolindolinone;

(d) $R_3$ is hydrogen;

(e) $R_4$, $R_5$, $R_6$, and $R_7$ are optionally present and are either (i) independently selected from the group consisting of hydrogen, alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, $SO_2NRR'$, $SO_3R$, SR, $NO_2$, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, $(CH_2)_nCO_2R$, and CONRR' or (ii) any two adjacent $R_4$, $R_5$, $R_6$, and $R_7$ taken together form a fused ring with the aryl portion of the oxindole-based portion of the indolinone;

(f) $R_2'$, $R_3'$, $R_4'$, $R_5'$, and $R_6'$ are each independently selected from the group consisting of hydrogen, alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, $SO_2NRR'$, $SO_3R$, SR, $NO_2$, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, $(CH_2)_nCO_2R$, and CONRR';

(g) n is 0, 1, 2, or 3;

(h) R is hydrogen, alkyl or aryl;

(i) R' is hydrogen, alkyl or aryl; and

(j) A is a five membered heteroaryl ring selected from the group consisting of thiophene, pyrrole, pyrazole, imidazole, 1,2,3-triazole, 1,2,4-triazole, oxazole, isoxazole, thiazole, isothiazole, furan, 1,2,3-oxadiazole, 1,2,4-oxadiazole, 1,2,5-oxadiazole, 1,3,4-oxadiazole, 1,2,3,4-oxatriazole, 1,2,3,5-oxatriazole, 1,2,3-thiadiazole, 1,2,4-thiadiazole, 1,2,5-thiadiazole, 1,3,4-thiadiazole, 1,2,3,4-thiatriazole, 1,2,3,5-thiatriazole, and tetrazole, optionally substituted at one or more positions with alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, $SO_2NRR'$, $SO_3R$, SR, $NO_2$, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, $(CH_2)_nCO_2R$ or CONRR'.

16. The crystalline form of claim 15, wherein said indolinone compound is 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone.

17. The crystalline form of claim 15, wherein said indolinone compound is 3-[4-(4-formylpiperazine-1-yl)benzylidenyl]-2-indolinone.

18. The crystalline form of claim 16, defined by the atomic structural coordinates of Table 3.

19. The crystalline form of claim 17, defined by the atomic structural coordinates of Table 4.

20. The crystalline form of claim 1, having monoclinic unit cells.

21. The crystalline form of claim 20, wherein said monoclinic unit cells have dimensions of about a=208.3 Å, b=57.8 Å, c=65.5 Å and β=107.2°.

22. The crystalline form of claim 20, wherein said monoclinic unit cells have dimensions of about a=211.6 Å, b=51.3 Å, c=66.1 Å and β=107.7°.

23. The crystalline form of claim 10, comprising one or more heavy metal atoms.

24. A polypeptide corresponding to the catalytic domain of a protein tyrosine kinase, containing at least about 20 amino acid residues upstream of the first

glycine in the conserved glycine-rich region of the catalytic domain, and at least about 17 amino acid residues downstream of the conserved arginine located at the C-terminal boundary of the catalytic domain.

25. The polypeptide of claim 24, wherein said protein tyrosine kinase is a receptor protein tyrosine kinase.

26. The polypeptide of claim 24, wherein said protein tyrosine kinase is a non-receptor protein tyrosine kinase.

27. The polypeptide of claim 25, wherein said receptor tyrosine kinase is selected from the group consisting of FGF-R, PDGF-R, KDR, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.

28. The polypeptide of claim 26, wherein said non-receptor kinase is selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

29. The polypeptide of claim 24 having the amino acid sequence shown in SEQ ID NO:4.

30. A method of using the polypeptide of claim 24 to form a crystal, comprising the steps of:

(a) mixing a volume of polypeptide solution with a reservoir solution; and

(b) incubating the mixture obtained in step (a) over the reservoir solution in a closed container, under conditions suitable for crystallization.

31. A method of obtaining an FGF receptor tyrosine kinase domain polypeptide in crystalline form, comprising the steps of:

(a) mixing a volume of polypeptide solution with an equal volume of reservoir solution, wherein said polypeptide solution comprises 1 mg/mL to 60 mg/mL FGF-type tyrosine kinase domain protein, 10 mM to 200 mM buffering agent, 0 mM to 20 mM dithiothreitol and has a pH of about 5.5 to about 7.5, and wherein said reservoir solution comprises 10% to 30% (w/v) polyethylene glycol, 0.1 M to 0.5 M ammonium sulfate, 0% to 20% (w/v) ethylene glycol or glycerol, 10 mM to 200 mM buffering agent and has a pH of about 5.5 to about 7.5; and

(b) incubating the mixture obtained in step (a) over said reservoir solution in a closed container at a temperature between 0° and 25° °C until crystals form.

32. The method of claim 31, wherein said polypeptide solution comprises about 10 mg/mL FGF receptor tyrosine kinase domain, about 10 mM sodium chloride, about 2 mM dithiothreitol, about 10 mM Tris-HCl and has a pH of about 8; the reservoir buffer comprises about 16% (w/v) polyethylene glycol (MW 10000), about 0.3 M ammonium sulfate, about 5% ethylene glycol or glycerol, about 100 mM bis-Tris and has a pH of about 6.5; and the temperature is about 4°C.

33. The method of claim 31, wherein said

polypeptide solution comprises a compound.

34. A cDNA encoding an FGF receptor tyrosine kinase domain protein, wherein a coding strand of the cDNA has the nucleotide sequence of SEQ ID NO:5.

35. A method of determining three dimensional structures of protein tyrosine kinases with unknown structure comprising the step of applying structural atomic coordinates set forth in Table 1, Table 2, Table 3, or Table 4.

36. The method of claim 35, comprising the following steps:

(a) aligning a first computer representation of an amino acid sequence of a protein tyrosine kinase of unknown structure with a second computer representation of a protein tyrosine kinase of known structure by matching homologous regions of amino acid sequences of said first computer representation and said second computer representation;

(b) transferring computer representations of amino acid structures in said protein tyrosine kinase of known structure to computer representations of corresponding amino acid structures in said protein tyrosine kinase with unknown structure; and

(c) determining a low energy conformation of the protein tyrosine kinase structure resulting from step (b).

37. The method of claim 35, comprising the

following steps:

(a) aligning the positions of atoms in the unit cell by matching electron diffraction data from two crystals; and

(b) determining a low energy conformation of the resulting protein tyrosine kinase structure.

38. The method of claim 35, comprising the following steps:

(a) determining the secondary structure of a protein tyrosine kinase structure using NMR data; and

(b) simplifying the assignment of through-space interactions of amino acids.

39. The method of any one of claims 35, 36, 37, or 38, wherein said protein tyrosine kinase with or without known structure is a receptor protein tyrosine kinase.

40. The method of claim 39, wherein said receptor protein tyrosine kinase with or without known structure is selected from the group consisting of FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.

41. The method of anyone of claims 35, 36, 37, or 38, wherein said protein tyrosine kinase with or without known structure is a non-receptor protein tyrosine kinase.

42. The method of claim 41, wherein said protein tyrosine kinase with or without known structure is

selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

43. A method of identifying a potential modulator of protein tyrosine kinase function by docking a computer representation of a structure of a compound with a computer representation of a structure of a cavity formed by the active-site of a protein tyrosine kinase, wherein said structure of said protein tyrosine kinase is defined by atomic structural coordinates set forth in Table 1, Table 2, Table 3, or Table 4.

44. The method of claim 43, comprising the following steps:

(a) removing a computer representation of a compound complexed with a protein tyrosine kinase and docking a computer representation of a compound from a computer data base with a computer representation of the active-site of the protein tyrosine kinase;

(b) determining a conformation of the complex resulting from step (a) with a favorable geometric fit and favorable complementary interactions; and

(c) identifying compounds that best fit said active-site as potential modulators of protein tyrosine kinase function.

45. The method of claim 43, comprising the following steps:

(a) modifying a computer representation of compound complexed with a protein tyrosine kinase by the deletion of a chemical group or groups or by the addition of a chemical group or groups;

(b) determining a conformation of the complex resulting from step (a) with a favorable geometric fit and favorable complementary interactions; and

(c) identifying compounds that best fit the protein tyrosine kinase active-site as potential modulators of protein tyrosine kinase function.

46. The method of claim 43, wherein said method comprises the following steps:

(a) removing a computer representation of a compound complexed with a protein tyrosine kinase; and

(b) searching a data base for data base compounds similar to said compounds using a compound searching computer program or replacing portions of said compound with similar chemical structures from a data base using a compound construction computer program.

47. The method of any one of claims 43, 44, 45, or 46, wherein said protein tyrosine kinase is a receptor protein tyrosine kinase.

48. The method of claim 47, wherein said receptor protein tyrosine kinase is selected from the group consisting of FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.

49. The method of anyone of claims 43, 44, 45, or 46, wherein said protein tyrosine kinase is a non-receptor protein tyrosine kinase.

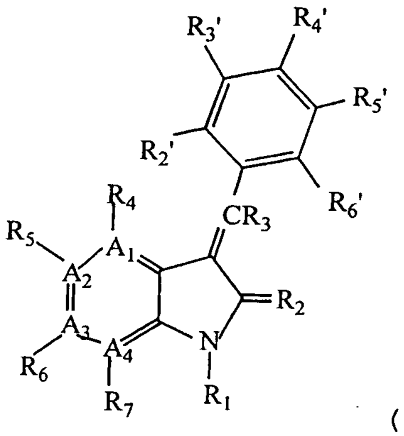
50. The method of claim 49, wherein said protein tyrosine kinase is selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

51. a potential modulator of protein tyrosine kinase function identified by the method of any one of claims 43, 44, 45, or 46.

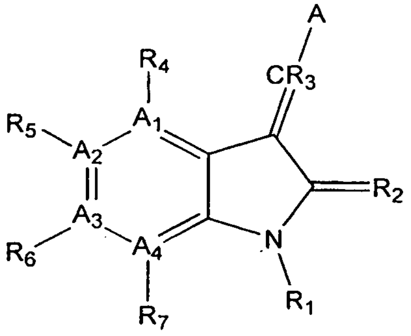
52. The potential modulator of claim 51, wherein said modulator is selected from a computer data base.

53. The potential modulator of claim 51, wherein said modulator is constructed from chemical groups selected from a computer data base.

54. The potential modulator of protein tyrosine kinase function of claim 51, wherein said modulator is an indolinone compound of formula I or II:



(I)



(II)

or a pharmaceutically acceptable salt, isomer, metabolite, ester, amide, or prodrug thereof, wherein

(a) $A_1$, $A_2$, $A_3$, and $A_4$ are independently carbon or nitrogen;

(b) $R_1$ is hydrogen or alkyl;

(c) $R_2$ is oxygen in the case of an oxindolinone or sulfur in the case of a thiolindolinone;

(d) $R_3$ is hydrogen;

(e) $R_4$, $R_5$, $R_6$, and $R_7$ are optionally present and are either (i) independently selected from the group consisting of hydrogen, alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, $SO_2NRR'$, $SO_3R$, SR, $NO_2$, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, $(CH_2)_nCO_2R$, and CONRR' or (ii) any two adjacent $R_4$, $R_5$, $R_6$, and $R_7$ taken together form a fused ring with the aryl portion of the oxindole-based portion of the indolinone;

(f) $R_2'$, $R_3'$, $R_4'$, $R_5'$, and $R_6'$ are each independently selected from the group consisting of hydrogen, alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, $SO_2NRR'$, $SO_3R$,

SR, $NO_2$, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, $(CH_2)_nCO_2R$, and CONRR';

(g) n is 0, 1, 2, or 3;

(h) R is hydrogen, alkyl or aryl;

(i) R' is hydrogen, alkyl or aryl; and

(j) A is a five membered heteroaryl ring selected from the group consisting of thiophene, pyrrole, pyrazole, imidazole, 1,2,3-triazole, 1,2,4-triazole, oxazole, isoxazole, thiazole, isothiazole, furan, 1,2,3-oxadiazole, 1,2,4-oxadiazole, 1,2,5-oxadiazole, 1,3,4-oxadiazole, 1,2,3,4-oxatriazole, 1,2,3,5-oxatriazole, 1,2,3-thiadiazole, 1,2,4-thiadiazole, 1,2,5-thiadiazole, 1,3,4-thiadiazole, 1,2,3,4-thiatriazole, 1,2,3,5-thiatriazole, and tetrazole, optionally substituted at one or more positions with alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, $SO_2NRR'$, $SO_3R$, SR, $NO_2$, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, $(CH_2)_nCO_2R$ or CONRR'.

55. A method of identifying a potential modulator of protein tyrosine kinase function as a modulator of protein tyrosine kinase function, comprising the following steps:

(a) administering said potential modulator to cells;

(b) comparing the level of protein tyrosine kinase phosphorylation between cells not administered the potential modulator and cells administered said potential modulator; and

(c) identifying said potential modulator as a modulator of protein tyrosine kinase function based on the difference in the level of protein tyrosine kinase phosphorylation.

56. A method of identifying a potential modulator of protein tyrosine kinase function as a modulator of protein tyrosine kinase function, wherein said method comprises the following steps:

(a) administering a preparation of said potential modulator to cells;

(b) comparing the rate of cell growth between cells not administered the modulator and cells administered the modulator; and

(c) identifying said potential modulator as a modulator of protein tyrosine kinase function based on the difference in the rate of cell growth.

57. A method of treating a disease associated with a protein tyrosine kinase with inappropriate activity in a cellular organism, wherein said method comprises the steps of:

(a) administering a modulator of protein tyrosine kinase function to the organism, wherein said modulator is in an acceptable pharmaceutical preparation; and

(b) activating or inhibiting the protein tyrosine kinase function to treat the disease.

58. The method of any one of claims 55, 56, or 57, wherein said protein tyrosine kinase is a receptor protein tyrosine kinase.

59. The method of claim 58, wherein said receptor protein tyrosine kinase is selected from the group containing FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.

60. The method of any one of claims 55, 56, or 57, wherein said protein tyrosine kinase is a non-receptor protein tyrosine kinase.

61. The method of claim 60, wherein said non-receptor protein tyrosine kinase is selected from a group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

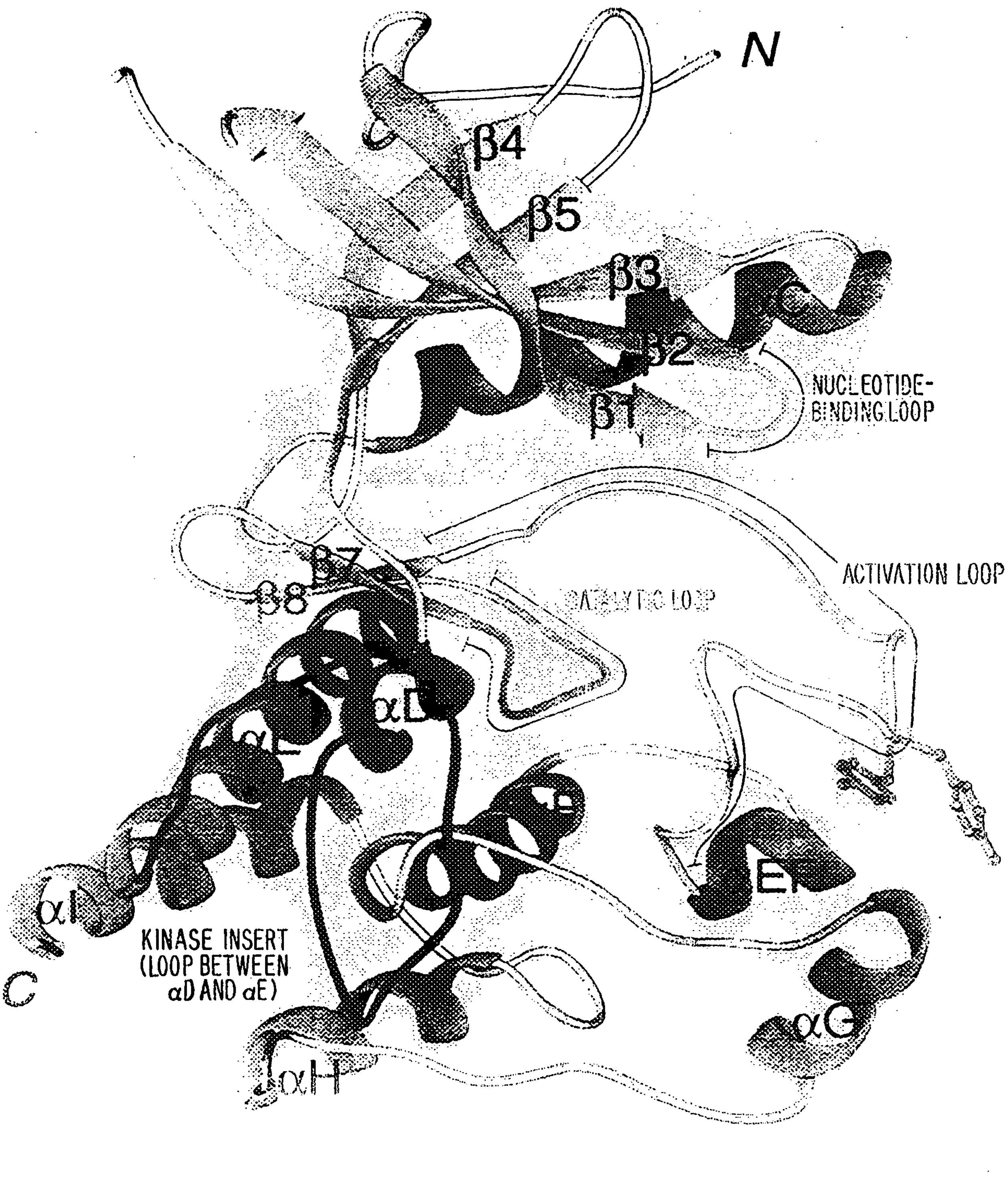


FIG. 1.

SUBSTITUTE SHEET (RULE 26)

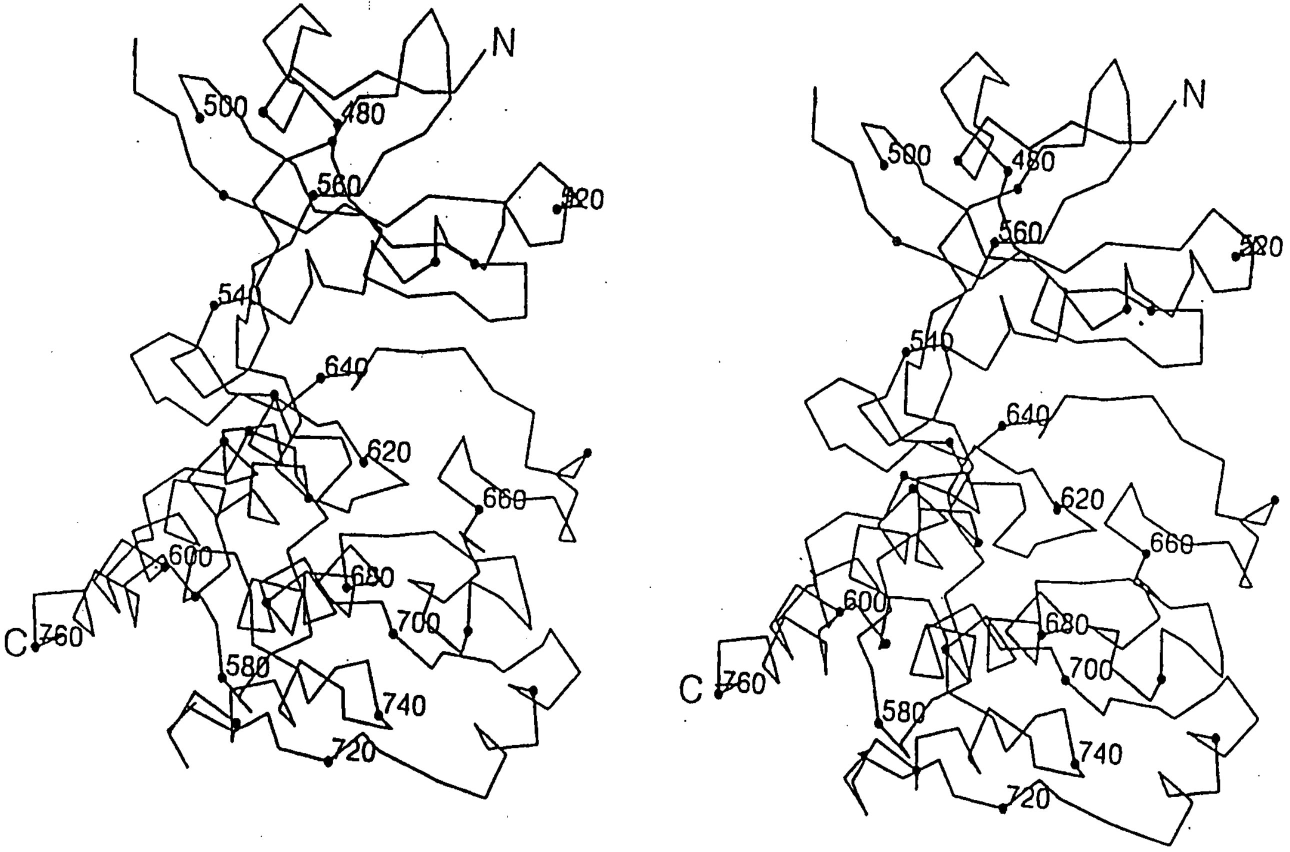


FIGURE 2

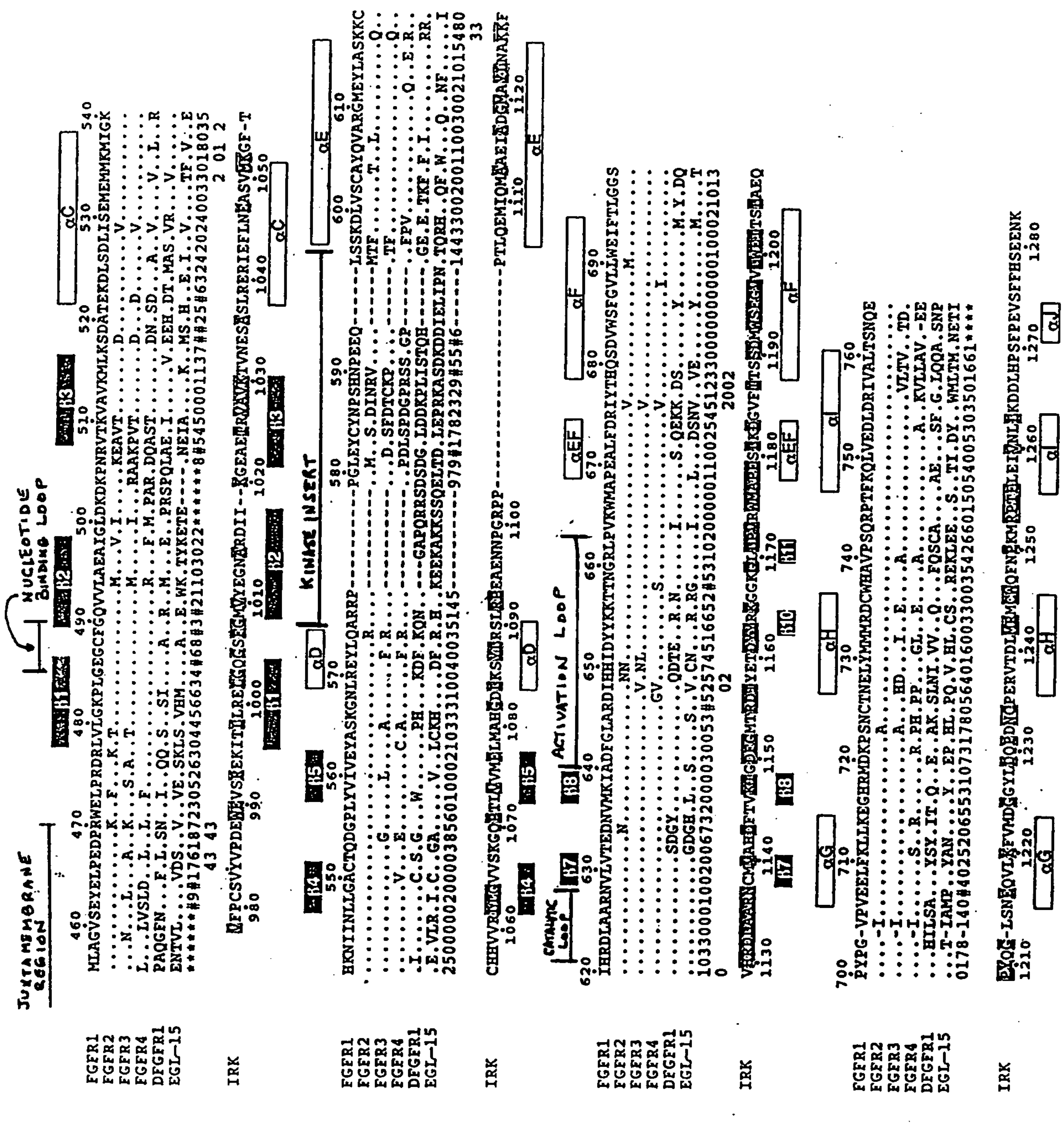
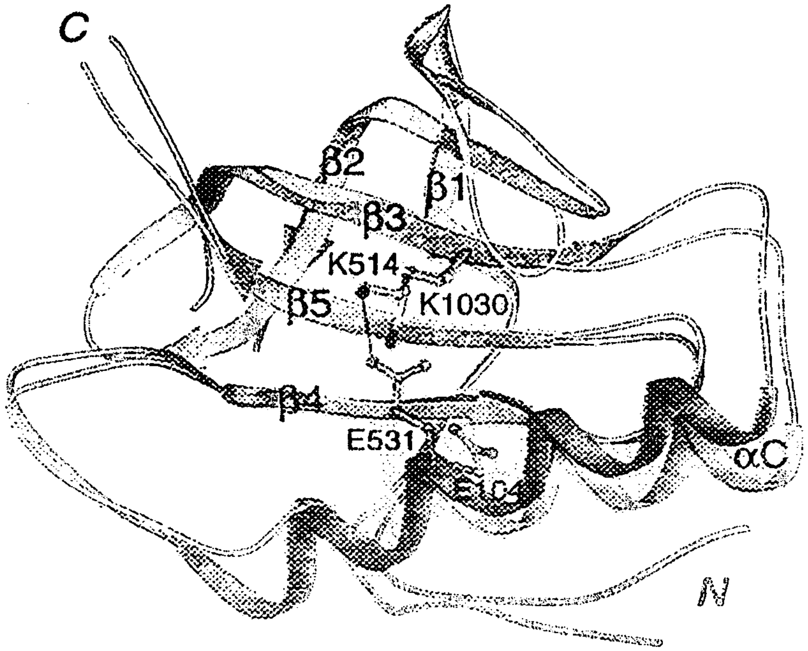

JUXTAMEMBRANE REGION
NUCLEOTIDE BINDING LOOP
KINASE INSERT
CATALYTIC LOOP
ACTIVATION LOOP
FGFR1
FGFR2
FGFR3
FGFR4
DFGFR1
EGL-15
IRK
β1
β2
β3
β4
β5
β7
β8
β10
β11
αC
αD
αE
αEF
αF
αG
αH
αI
αJ

FIGURE 3

FIG. 4A.


C
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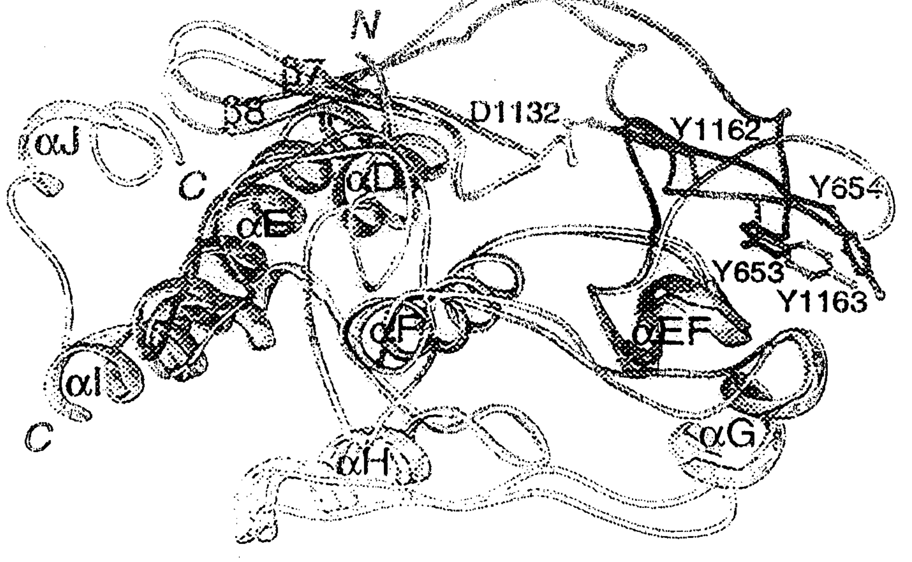
β1
β3
K514
K1030
β5
β4
E531
E10
αC
N

FIG. 4B.


N
β7
β8
D1132
Y1162
αJ
C
αD
αE
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Y653
Y1163
αF
αEF
αI
C
αG
αH

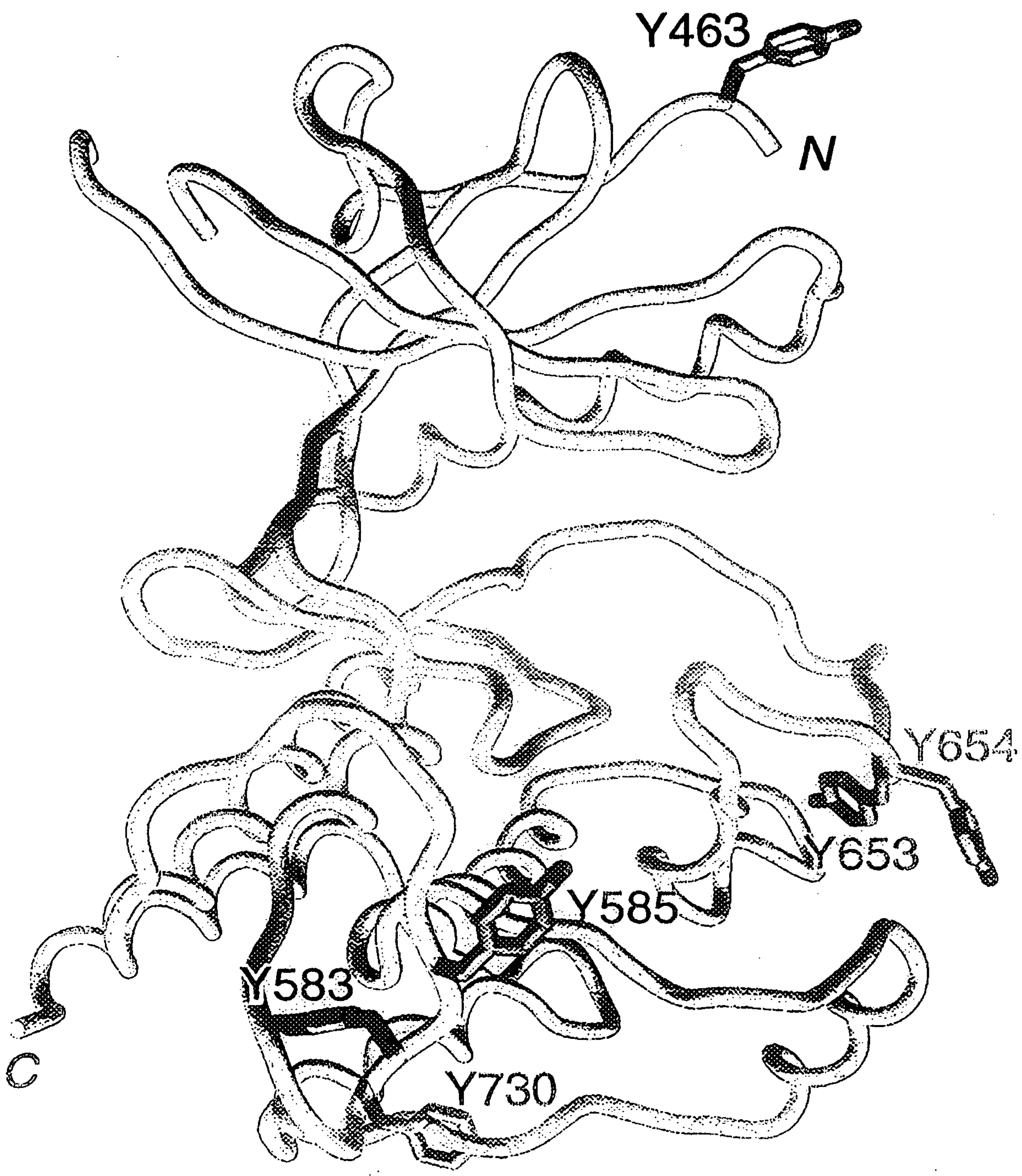

*FIG. 5.*

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                                  GLYCINE
                                     RICH
                                    |-----|
          466
FGFR1_h   LP-ED-PRW- E--LPRDRLV LGKPLGEGCF GQVVLAEAIG LDK-DK---- ------PNRV TKVAVKMLKS -DATEKDLSD LISEMEMMKM
 EGFR_h   PNQALLRILK ETEFKKIKV- ----LGSGAF GTVYKGLWIP E-G-EK---- -------V-K IPVAIKELRE -ATSPKANKE ILDEAYVMAS
 INSR_h   VYVPDE--W- E--VSREKIT LLRELGQGSF GMVYEGNARD IIK-GE---- -------A-E TRVAVKTVNE -SASLRERIE FLNEASVMKG
PDGFRa_h  LP-YD-SRW- E--FPRDGLV LGRVLGSGAF GKVVEGTAYG LSR-SQ---- -------P-V MKVAVKMLKP -TARSSEKQA LMSELKIMTH
  KDR_h   -P-YDASKW- E--FPRDRLN LGKPLGRGAF GQEIEADAFG IDK-TA---- -------T-C RTVAVKMLKE -GATHSEHRA LMSELKILIH
 CCK4_h   HSTSD--KM- H--FPRSSLQ PITTLGKSEF GEVFLAKAQG LEE-GV---- -------A-E TLVLVKSLQ- -SKDEQQQLD FRRELEMFGK
  MET_h   AVQHVVIGPS SLI-----VH FNEVIGRGHF GCVYHGTLLD N-D-GK---- ---------K IHCAVKSLNR -ITDIGEVSQ FLTEGIIMKD
 TRKA_h   FSDACVHHIK -----RRDIV LKWELGEGAF GKVFLAECHN LLP-EQ---- -------D-K MLVAVKALK- -EASESARQD FQREAELLTM
  AXL_h   --KEKL--R- DVMVDRHKVA LGKTLGEGEF GAVMEGQLNQ D-D-SI---- ---------- LKVAVKTMKI AICTRSELED FLSEAVCMKE
  TIE_h   -P-EPL--S- YPVLEWEDIT FEDLIGEGNF GQVIRAMIKK D-GLK----- ---------- MNAAIKMLKE -YASENDHRD FAGELEVLCK
  EPH_h   WSNFPS--R- E--LDPAWLM VDTVIGEGEF GEVYRGTLRL P-S-QD---- ---------C KTVAIKTLKD -TSPGGQWWN FLREATIMGQ
  RYK_h   --KGKV--K- DIAISRERIT LKDVLQEGTF GRIFHGILID EKD-PN---- -------K-E KQAFVKTVKD -QASEIQVTM MLTESCKLRG
  DDR_h   GDG-P-PRV- D--FPRSRLR FKEKLGEGQF GEVHLCEVDS PQD-LVSLDF PLNVRKGH-P LLVAVKILRP -DATKNARND FLKEVKIMSR
  ROS_h   E--EIE--N- LPAFPREKLT LRLLLGSGAF GEVYEGTAVD ILGVGS---- -------G-E IKVAVKTLKK -GSTDQEKIE FLKEAHLMSK
  RET_h   IL-ED-PKW- E--FPRKNLV LGKTLGEGEF GKVVKATAFH LKG-RA---- -------G-Y TTVAVKMLKE -NASPSELRD LLSEFNVLKQ
  LTK_h   -P-LP-PGVT E--VSPANVT LLRALGHGAF GEVYEGLVIG LPG-DS---- -------S-P LQVAIKTLPE -LCSPQDELD FLMEALIISK
 ROR1_h   KPKSKA--K- E--LPLSAVR FMEELGECAF GKIYKGHLYL P-G-MD---- -------H-A QLVAIKTLKD -YNNPQQWME FQQEASLMAE
 MUSK_m   NPKLLS--L- E--YPRNNIE YVRDIGEGAF GRVFQARAPG LLP-YE---- -------P-F TMVAVKMLKE -EASADMQAD FQREAALMAE
                                     I                                          II                   III
```

Fig. 6A-1

```
          538                |------------------------  KINASE INSERT  ------------------------------|
 FGFR1_h  IGKHKNIINL LGACTQD-GP L-----YVIV EYASKGNLRE YLQ-ARRPPG LEYCYNPSH- ---------- ---NP---E- -EQL-SSKDL
  EGFR_h  VDN-PHVCRL LGICLTS-TV Q-----LI-T QLMPFGCLLD YVR-EHK-DN ---------- ---------- ---------- ---IGSQY-L
  INSR_h  FTC-HHVVRL LGVVSKG-QP T-----LVVM ELMAHGDLKS YLR-SLRP-- --------EA ENN------- PG------R- -PPP-TLQEM
PDGFRa_h  LGPHLNIVNL LGACTKS-GP I-----YIIT EYCFYGDLVN YLH-KNR-DS F---L--SH- ---------- ---HPE(87) SEGL-TLLDL
   KDR_h  IGHHLNVVNL LGACTKPGGP L-----MVIV EFCKFGNLST YLR-SKR-NE F---V--PY- ---------- ---KTK(55) KDFL-TLEHL
  CCK4_h  LNH-ANVVRL LGLCREA-EP H-----YMVL EYVDLGDLKQ FLRISKSKDE K---L----- ---------- ----K---S- -QPL-STKQK
   MET_h  FSH-PNVLSL LGICLRS-EG ----SPLVVL PYMKHGDLRN FIR-NE---- ---------T HN-------- ---------- ---P-TVKDL
  TRKA_h  LQH-QHIVRF FGVCTEG-RP L-----LMVF EYMRHGDLNR FLR-SHGPDA K---LLAGGE DVA------- --------P- -GPL-GLGQL
   AXL_h  FDH-PNVMRL IGVCFQGSER ESFPAPVVIL PFMKHGDLHS FLLYSRLGD- ---------- ---------- ----Q---P- -VYL-PTQML
   TIE_h  LGHHPNIINL LGACKNR-GY L-----YIAI EYAPYGNLLD FLR-KSRVLE TDPAFAREH- ---------- ---GT---A- -STL-SSRQL
   EPH_h  FSH-PHILHL EGVVTKR-KP I-----MIIT EFMENGALDA FLR-ERE-DQ ---------- ---------- ---------- ---L-VPGQL
   RYK_h  LHH-RNLLPI THVCIEE-GE ----KPMVIL PYMNWGNLKL FLRQ------ --CKL--VEA NN-------- --------P- -QAI-SQQDL
   DDR_h  LKD-PNIIRL LGVCVQD-DP L-----CMIT DYMENGDLNQ FLS-AHQLED KA-------A EGA------- PGDGQAAQG- -PTI-SYPML
   ROS_h  FNH-PNILKQ LGVCLLN-EP Q-----YIIL ELMEGGDLLT YLR-KARM-A ---------- ---------- --TFY---G- -PLL-TLVDL
   RET_h  VNH-PHVIKL YGACSQD-GP L-----LLIV EYAKYGSLRG FLR-ESRKVG PGYLGSGGSR NSSSLDHPDE RA-------- ---L-TMGDL
   LTK_h  FRH-QNIVRC VGLSLRA-TP R-----LILL ELMSGGDMKS FLR-HSRP-H ---------- ---------- --LGQ---P- -SPL-VMRDL
  ROR1_h  LHH-PNIVCL LGAVTQE-QP V-----CMLF EYINQGDLHE FLI-MRSP-H SDVGCSSDED GTVK------ ---------- -SSL-DHGDF
  MUSK_m  FDN-PNIVKL LGVCAVG-KP M-----CLLF EYMAYGDLNE FLR-SMSP-H TVCSL--SHS DLSTRARVSS PG------P- -PPL-SCAEQ
                         IV                     V                                                       VIa
```

Fig. 6A-2

```
                               CATALYTIC
                                  LOOP                           ACTIVATION LOOP
          601                   |------|                   |--------------------------|
FGFR1_h   VSCAYQVARG MEYLASKKCI HRDLAARNVL VTED-----N VMKIADFGLA RDIHHIDYYK K--TTNGRLP VKWMAPEALF DRIYTHQSDV
  EGFR_h  LNWCVQIAKG MNYLEDRRLV HRDLAARNVL VKTP-----Q HVKITDFGLA KLLGAEEKEY H--AEGGKVP IKWMALESIL HRIYTHQSDV
  INSR_h  IQMAAEIADG MAYLNAKKFV HRDLAARNCM VAHD-----F TVKIGDFGMT RDIYETDYYR K--GGKGLLP VRWMAPESLK DGVFTTSSDM
PDGFRa_h  LSFTYQVARG MEFLASKNCV HRDLAARNVL LAQG-----K IVKICDFGLA RDIMHDSNYV S--KGSTFLP VKWMAPESIF DNLYTTLSDV
   KDR_h  ICYSFQVAKG MEFLASRKCI HRDLAARNIL LSEK-----N VVKICDFGLA RDIYKDPDYV R--KGDARLP LKWMAPETIF DRVYTIQSDV
  CCK4_h  VALCTQVALG MEHLSNNRFV HKDLAARNCL VSAQ-----R QVKVSALGLS KDVYNSEYYH FRQAWV---P LRWMSPEAIL EGDFSTKSDV
   MET_h  IGFGLQVAKG MKYLASKKFV HRDLAARNCM LDEK-----F TVKVADFGLA RDMYDKEYYS VHNKTGAKLP VKWMALESLQ TQKFTTKSDV
  TRKA_h  LAVASQVAAG MVYLAGLHFV HRDLATRNCL VGQG-----L VVKIGDFGMS RDIYSTDYYR V--GGRTMLP IRWMPPESIL YRKFTTESDV
   AXL_h  VKFMADIASG MEYLSTKRFI HRDLAARNCM LNEN-----M SVCVADFGLS KKIYNGDYYR Q--GRIAKMP VKWIAIESLA DRVYTSKSDV
   TIE_h  LRFASDAANG MQYLSEKQFI HRDLAARNVL VGEN-----L ASKIADFGLS R--G-EEVYV K--KTMGRLP VRWMAIESLN YSVYTTKSDV
   EPH_h  VAMLQGIASG MNYLSNHNYV HRDLAARNIL VNQN-----L CCKVSDFGLT RLLDDFDGTY E--TQGGKIP IRWTAPEAIA HRIFTTASDV
   RYK_h  VHMAIQIACG MSYLARREVI HKDLAARNCV IDDT-----L QVKITDNALS RDLFPMDYHC L--GDNENRP VRWMALESLV NNEFSSASDV
   DDR_h  LHVAAQIASG MRYLATLNFV HRDLATRNCL VGEN-----F TIKIADFGMS RNLYAGDYYR V--QGRAVLP IRWMAWECIL MGKFTTASDV
   ROS_h  VDLCVDISKG CVYLERMHFI HRDLAARNCL VSVKDYTSPR IVKIGDFGLA RDIYKNDYYR K--RGEGLLP VRWMAPESLM DGIFTTQSDV
   RET_h  ISFAWQISQG MQYLAEMKLV HRDLAARNIL VAEG-----R KMKISDFGLS RDVYEEDSYV K--RSQGRIP VKWMAIESLF DHIYTTQSDV
   LTK_h  LQLAQDIAQG CHYLEENHFI HRDIAARNCL LSCAGPS--R VAKIGDFGMA RDIYRASYYR R--GDRALLP VKWMPPEAFL EGIFTSKTDS
  ROR1_h  LHIAIQIAAG MEYLSSHFFV HKDLAARNIL IGEQ-----L HVKISDLGLS REIYSADYYR V--QSKSLLP IRWMPPEAIM YGKFSSDSDI
  MUSK_m  LCIARQVAAG MAYLSERKFV HRDLATRNCL VGET-----M VVKIADFGLS RNIYSADYYK A--DGNDAIP IRWMPPESIF YNRYTTESDV
                           VIb                             VII                               VIII        IX
```

Fig. 6A-3

```
          684                                                                                                 763
FGFR1_h   WSFGV-LLWE IFTLGG-SPY P-GVPVEE-- ----LF-KLL KEGHRMDKPS NCTNELYMMM RDCWHAVPSQ RPTFKQLVED LDRIVALTSN
 EGFR_h   WSYGV-TVWE LMTFGS-KPY D-GIPASE-- ----IS-SIL EKGERLPQPP ICTIDVYMIM VKCWMIDADS RPKFRELIIE FSKMARDPQR
 INSR_h   WSFGV-VLWE ITSLAE-QPY Q-GLSNEQ-- ----VL-KFV MDGGYLDQPD NCPERVTDLM RMCWQFNPKM RPTFLEIVNL LKDDLHPSFP
PDGFRa_h  WSYGI-LLWE IFSLGG-TPY P-GMMVDS-- ----TFYNKI KSGYRMAKPD HATSEVYEIM VKCWNSEPEK RPSFYHLSEI VENLLPGQYK
  KDR_h   WSFGV-LLWE IFSLGA-SPY P-GVKIDE-- ----EFCRRL KEGTRMRAPD YTTPEMYQTM LDCWHGEPSQ RPTFSELVEH LGNLLQANAQ
 CCK4_h   WAFGV-LMWE VFTHGE-MPH G-GQADDE-- ----VLADLQ AGKARLPQPE GCPSKLYRLM QRCWALSPKD RPSFSEIASA LGDSTVDSKP
  MET_h   WSFGV-VLWE LMTRGA-PPY P-DVNTFD-- ----IT-VYL LQGRRLLQPE YCPDPLYEVM LKCWHPKAEM RPSFSELVSR ISAIFSTFIG
 TRKA_h   WSFGV-VLWE IFTYGK-QPW Y-QLSNTE-- ----AI-DCI TQGRELERPR ACPPEVYAIM RGCWQREPQQ RHSIKDVHAR LQALAQAPPV
  AXL_h   WSFGV-TMWE IATRGQ-TPY P-GVENSE-- ----IY-DYL RQGNRLKQPA DCLDGLYALM SRCWELNPQD RPSFTELRED LENTLKALPP
  TIE_h   WSFGV-LLWE IVSLGG-TPY C-GMTCAE-- ----LY-EKL PQGYRMEQPR NCDDEVYELM RQCWRDRPYE RPPFAQIALQ LGRMLEARKA
  EPH_h   WSFGI-VMWE VLSFGD-KPY G-EMSNQE-- ----VM-KSI EDGYRLPPPV DCPAPLYELM KNCWAYDRAR RPHFQKLQAH LEQLLANPHS
  RYK_h   WAFGVNSLWE LMTLGQ-TPY TLDIDPFE-- ----MAA-YL KDGYRIAQPI TCPDELFAVM ACCWALDPEE RPRFQQLVQC LTEFHAALGA
  DDR_h   WAFGV-TVWE VLMLCRAQPF G-QLTDEQVI ENAGEFFRDQ GRQVYLSRPP ACPQGLYELM LRCWSRESEQ RPPFSQLHRF LAEDALNTV-
  ROS_h   WSFGI-LIWE ILTLGH-QPY P-AHSNLD-- ----VL-NYV QTGGRLEPPR NCPDDLWNLM TQCWAQEPDQ RPTFHRIQNQ LQLFRNFFLN
  RET_h   WSFGV-LLWE IVTLGG-NPY P-GIPPER-- ----LF-NLL KTGHRMERPD NCSEEMYRLM LQCWKQEPDK RPVFADISKD LEKMMVKRRD
  LTK_h   WSFGV-LLWE IFSLGY-MPY P-GRTNQE-- ----VL-DFV VGGGRMDPPR GCPGPVYRIM TQCWQHEPEL RPSFASILER LQYCTQDPDV
 ROR1_h   WSFGV-VLWE IFSFGL-QPY Y-GFSNQE-- ----VI-EMV RKRQLLPCSE DCPPRMYSLM TECWNEIPSR RPRFKDIHVR LRSWEGLSSH
 MUSK_m   WAYGV-VLWE IFSYGL-QPY Y-GMAHEE-- ----VI-YYV RDGNILACPE NCPLELYNLM RLCWSKLPAD RPSFCSIHRI LQRMCERAEG
                                 X                                    XI
```

Fig. 6A-4

```
           465
FGFR1_h    LPEDPRWELP RDRLVLGK-P LGEGCFGQVV LAEAIGLDKD KPNRVTKVAV KMLKSDATEK DLSDLISEME MMKMI-GKHK
  SRC_h    GLAKDAWEIP RESLRLEV-K LGQGCFGEVW MGTW------ NGT--TRVAI KTLKPGTMSP -E--AFLQ-E AQVMKKLRHE
  BRK_h    LPHWDDWERP REEFTLCR-K LGSGYFGEVF EGLW------ KDR--VQVAI KVISRDNLLH -Q--QMLQSE IQAMKKLRHK
  BTK_h    GLGYGSWEID PKDLTFLK-E LGTGQFGVVK YGKW------ RGQYD--VAI KMIKEGSMSE -D--EFIE-E AKVMMNLSHE
  CSK_h    EFYRSGWALN MKELKLLQ-T IGKGEFGDVM LGDY------ RGN---KVAV KCIKNDA-TA -Q--AFL-AE ASVMTQLRHS
  ABL_h    SPNYDKWEME RTDITMKH-K LGGGQYGEVY EGVW------ K-KYSLTVAV KTLKEDTMEV -E--EFLK-E AAVMKEIKHP
ZAP70_h    LKDKKLF-LK RDNLLIADIE LGCGNFGSVR QGVY----RM RKKQ-IDVAI KVLKQG--TE KADTEEMMRE AQIMHQLDNP
  FES_h    AVPKDKWVLN HEDLVLGE-Q IGRGNFGEVF SGR------- LRADNTLVAV KSCRETLPPD LKAK-FLQ-E ARILKQYSHP
  FAK_h    MPSTRDYEIQ RERIELGRC- IGEGQFGDVH QGIY----MS PENPALAVAI KTCKNC--TS DSVREKFLQE ALTMRQFDHP
 JAK1_h    PTEVDPTHFE KRFLKRIR-D LGEGHFGKVE LCRY----DP EDNTGEQVAV KSLKPE--SG GNHIADLKKE IEILRNLYHE
  ACK_h    PLQSLTCLIG EKDLRLLE-K LGDGSFGVVR RGEW----DA PSGKTVSVAV KCLKPDVLSQ PEAMDDFIRE VNAMHSLDHR
                                   I                     II                     III

           543
FGFR1_h    NIINLLGACT -QDGP-LYVI VEYASKGNLR EYLQARRPPG LEYCYNPSHN PEEQLSSKDL VSCAYQVARG MEYLASKKCI
  SRC_h    KLVQLYAVVS -E-EP-IYIV TEYMSKGSLL DFLKGET--- ---------- -GKYLRLPQL VDMAAQIASG MAYVERMNYV
  BRK_h    HILALYAVVS VG-DP-VYII TELMAKGSLL ELLRDSD--- ---------- -EKVLPVSEL LDIAWQVAEG MCYLESQNYI
  BTK_h    KLVQLYGVCT KQR-P-IFII TEYMANGCLL NYLRE-M--- ---------- -RHRFQTQQL LEMCKDVCEA MEYLESKQFL
  CSK_h    NLVQLLGVIV EEKGG-LYIV TEYMAKGSLV DYLRSRG--- ---------- -RSVLGGDCL LKFSLDVCEA MEYLEGNNFV
  ABL_h    NLVQLLGVCT REP-P-FYII TEFMTYGNLL DYLRECN--- ---------- -RQEVNAVVL LYMATQISSA MEYLEKKNFI
ZAP70_h    YIVRLIGVCQ AEA---LMLV MEMAGGGPLH KFLVGK---- ---------- -REEIPVSNV AELLHQVSMG MKYLEEKNFV
  FES_h    NIVRLIGVCT -QKQP-IYIV MELVQGGDFL TFLRTE---- ---------- -GARLRVKTL LQMVGDAAAG MEYLESKCCI
  FAK_h    HIVKLIGVIT ENP---VWII MELCTLGELR SFLQVR---- ---------- -KYSLDLASL ILYAYQLSTA LAYLESKRFV
 JAK1_h    NIVKYKGICT EDGGNGIKLI MEFLPSGSLK EYLPKN---- ---------- -KNKINLKQQ LKYAVQICKG MDYLGSRQYV
  ACK_h    NLIRLYGVVL TPP---MKMV TELAPLGSLL DRLRKH---- ---------- -QGHFLLGTL SRYAVQVAEG MGYLESKRFI
                  IV                    V                                VIa                VIb
```

Fig. 6B-1

```
           621
FGFR1_h    HRDLAARNVL VTEDNVMKIA DFGLARDIH- HIDYYKKTTN GRLPVKWMAP EAL-FDRIYT HQSDVWSFGV LLWEIFTLGG
  SRC_h    HRDLRAANIL VGENLVCKVA DFGLARLIE- DNEYTARQGA -KFPIKWTAP EAALYGR-FT IKSDVWSFGI LLTELTTKGR
  BRK_h    HRDLAARNIL VGENTLCKVG DFGLARLIK- EDVYLSHD-H -NIPYKWTAP EALSRGH-YS TKSDVWSFGI LLHEMFSRGQ
  BTK_h    HRDLAARNCL VNDQGVVKVS DFGLSRYVL- DDEYTSSVGS -KFPVRWSPP EVLMYSK-FS SKSDIWAFGV LMWEIYSLGK
  CSK_h    HRDLAARNVL VSEDNVAKVS DFGLTK---- -EASSTQDTG -KLPVKWTAP EALREKK-FS TKSDVWSFGI LLWEIYSFGR
  ABL_h    HRDLAARNCL VGENHLVKVA DFGLSRLMT- GDTYTAHAGA -KFPIKWTAP ESLAYNK-FS IKSDVWAFGV LLWEIATYGM
ZAP70_h    HRDLAARNVL LVNRHYAKIS DFGLSKALGA DDSYYTARSA GKWPLKWYAP ECINFRK-FS SRSDVWSYGC TMWEALSYGQ
  FES_h    HRDLAARNCL VTEKNVLKIS DFGMSREEA- DGVYAASGGS RQVPVKWTAP EALNYGR-YS SESDVWSFGI LLWETFSLGA
  FAK_h    HRDIAARNVL VSSNDCVKLG DFGLSRYME- DSTYYKA-SK GKLPIKWMAP ESINFRR-FT SASDVWMFGV CMWEILMHGV
 JAK1_h    HRDLAARNVL VESEHQVKIG DFGLTKAIET DKEYYTVKDD RDSPVFWYAP ECLMQSK-FY IASDVWSFGV TLHELLTYCD
  ACK_h    HRDLAARNLL LATRDLVKIG DFGLMRALPQ NDDHYVMQEH RKVPFAWCAP ESLKTRT-FS HASDTWMFGV TLWEMFTYGQ
                                 VII                                     VIII         IX

           699                                                                                764
FGFR1_h    S--------- ----PYPGVP VEELFKLLKE -GHRMDKPSN CTNELYMMMR DCWHAVPSQR PTFKQLVEDL DRIVALTSNQ
  SRC_h    V--------- ----PYPGMV NREVLDQVER -GYRMPCPPE CPESLHDLMC QCWRKEPEER PTFEYLQAFL EDYFTSTEPQ
  BRK_h    V--------- ----PYPGMS NHEAFLRVDA -GYRMPCPLE CPPSVHKLML TCWCRDPEQR PCFKALRERL SSFTSYENPT
  BTK_h    M--------- ----PYERFT NSETAEHIAQ -GLRLYRPHL ASEKVYTIMY SCWHEKADER PTFKILLSNI LDVMDEES--
  CSK_h    V--------- ----PYPRIP LKDVVPRVEK -GYKMDAPDG CPPAVYEVMK NCWHLDAAMR PSFLQLREQL EHIKTHELHL
  ABL_h    S--------- ----PYPGID LSQVYELLEK -DYRMERPEG CPEKVYELMR ACWQWNPSDR PSFAEIHQAF ETMFQESSIS
ZAP70_h    K--------- ----PYKKMK GPEVMAFIE- QGKRMECPPE CPPELYALMS DCWIYKWEDR PDFLTVEQRM RACYYSLASK
  FES_h    S--------- ----PYPNLS NQQTREFVEK -GGRLPCPEL CPDAVFRLME QCWAYEPGQR PSFSTIYQEL QSIR--KRHR
  FAK_h    K--------- ----PFQGVK NNDVIGRIE- NGERLPMPPN CPPTLYSLMT KCWAYDPSRR PRFTELKAQL STILEEEKAQ
 JAK1_h    SDSSPMALFL KMIGPTHGQM TVTRLVNTLK EGKRLPCPPN CPDEVYQLMR KCWEFQPSNR TSFQNLIEGF -----EALLK
  ACK_h    E--------- ----PWIGLN GSQILHKIDK EGERLPRPED CPQDIYNVMV QCWAHKPEDR PTFVALRDFL LEAQPTDMRA
                          X                                      XI
```

Fig. 6B-2

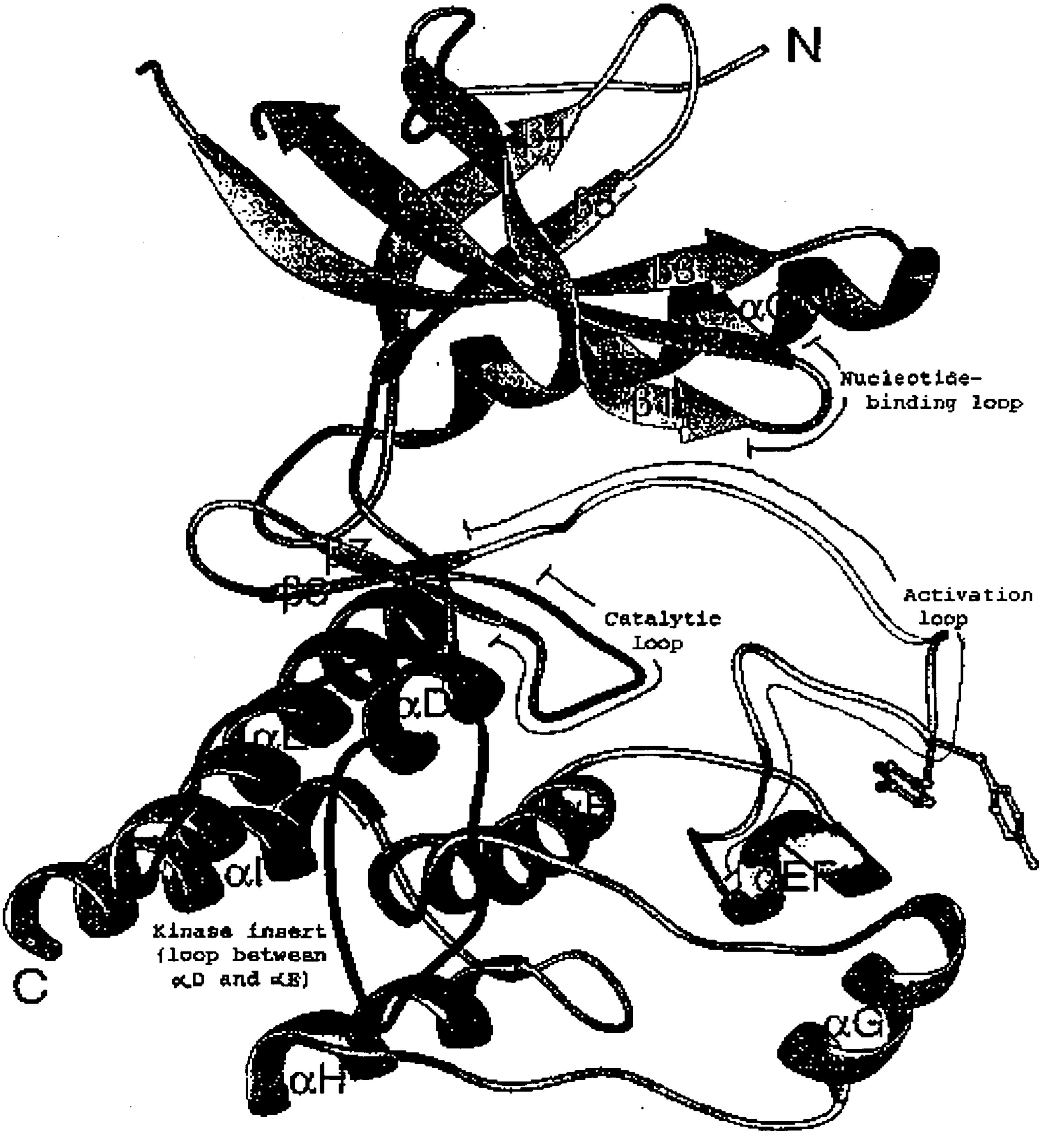

N
β4
β5
β3
β2
αC
Nucleotide-binding loop
β1
β7
β6
Catalytic Loop
Activation loop
αD
αE
αF
αI
αEF
Kinase insert (loop between αD and αE)
C
αG
αH

FIGURE 1

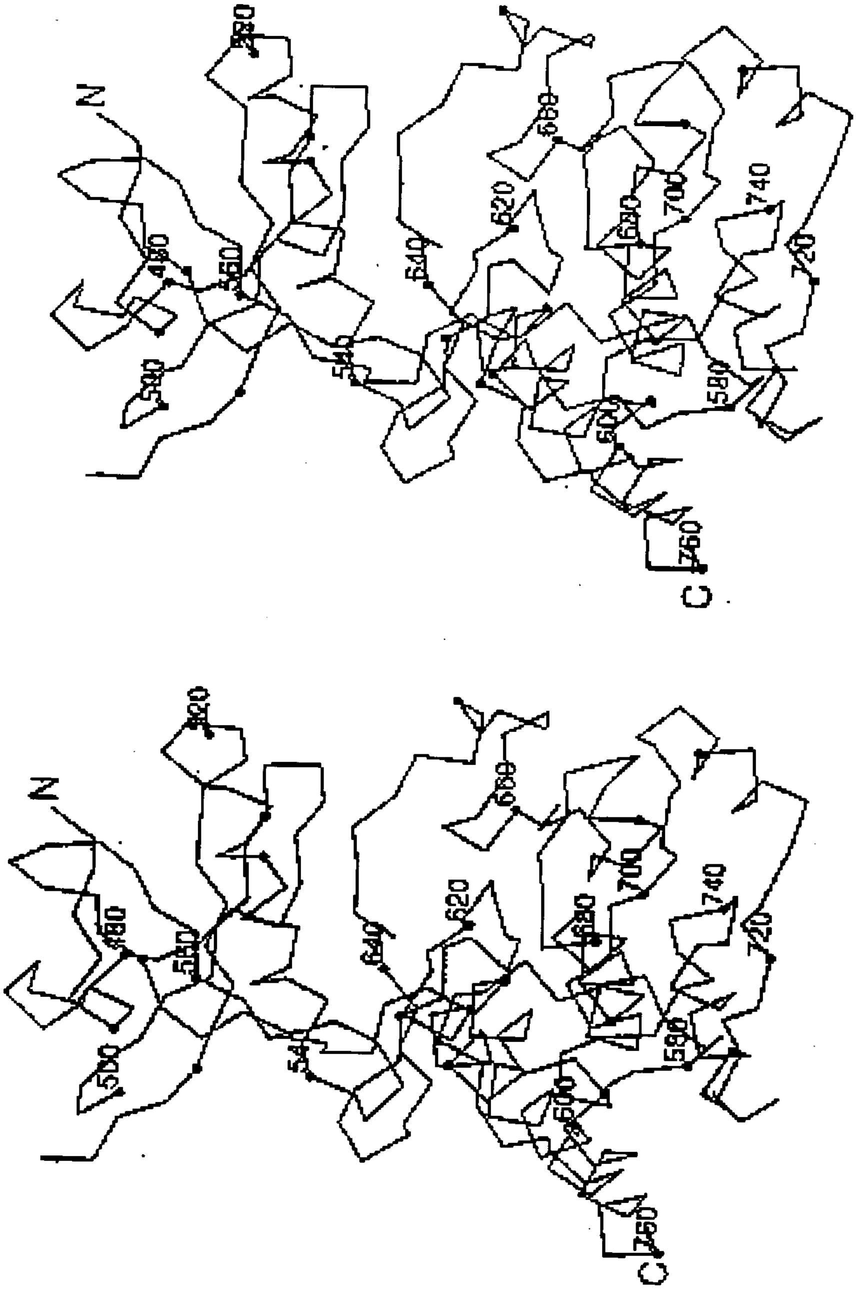


FIGURE 2

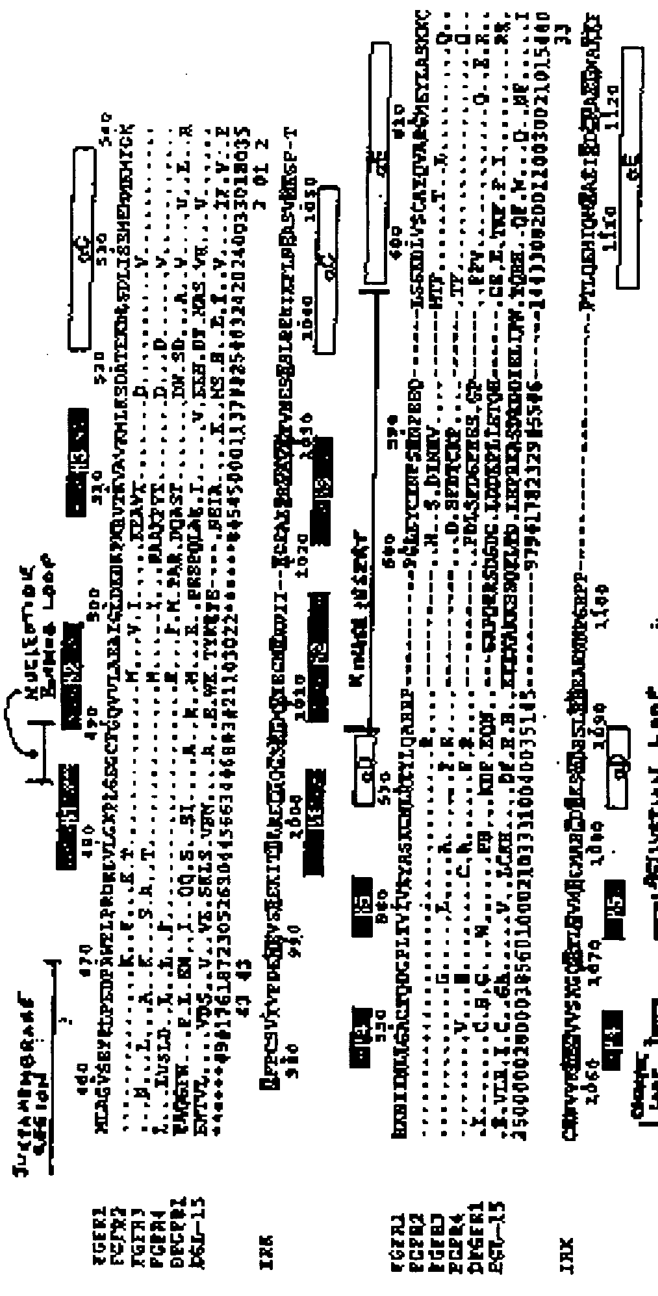

Juxtamembrane region
Nucleotide binding loop
Catalytic loop
Activation loop
FGFR1
FGFR2
FGFR3
FGFR4
DFGFR1
EGL-15
IRK

FIGURE 3

FIGURE 4A

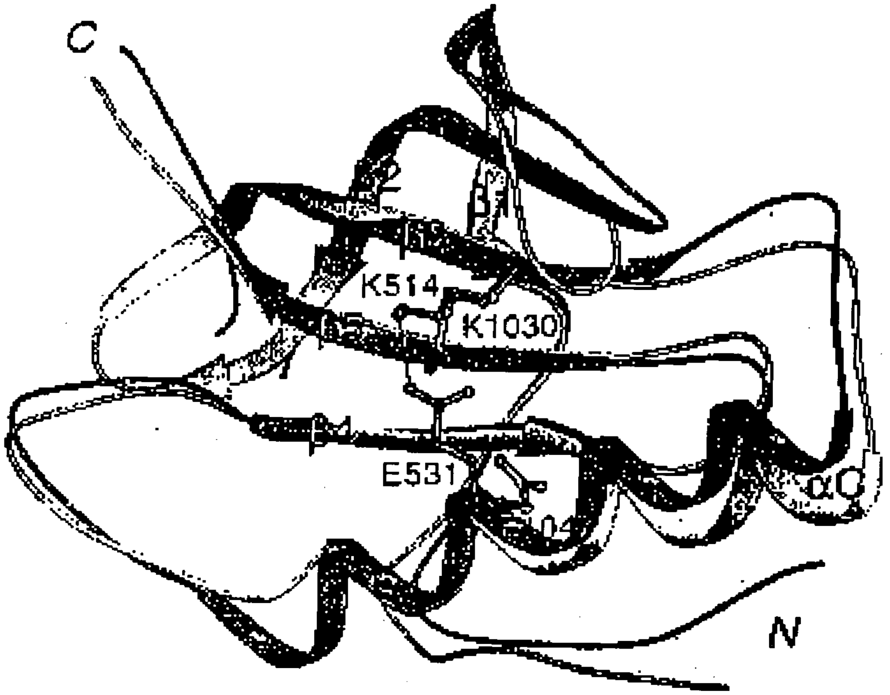
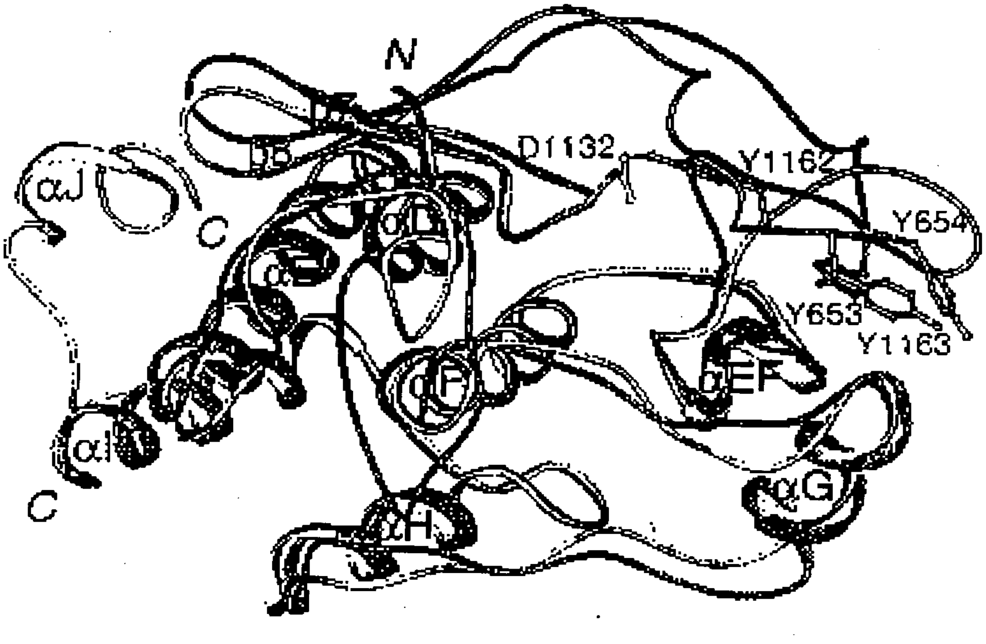


FIGURE 4B



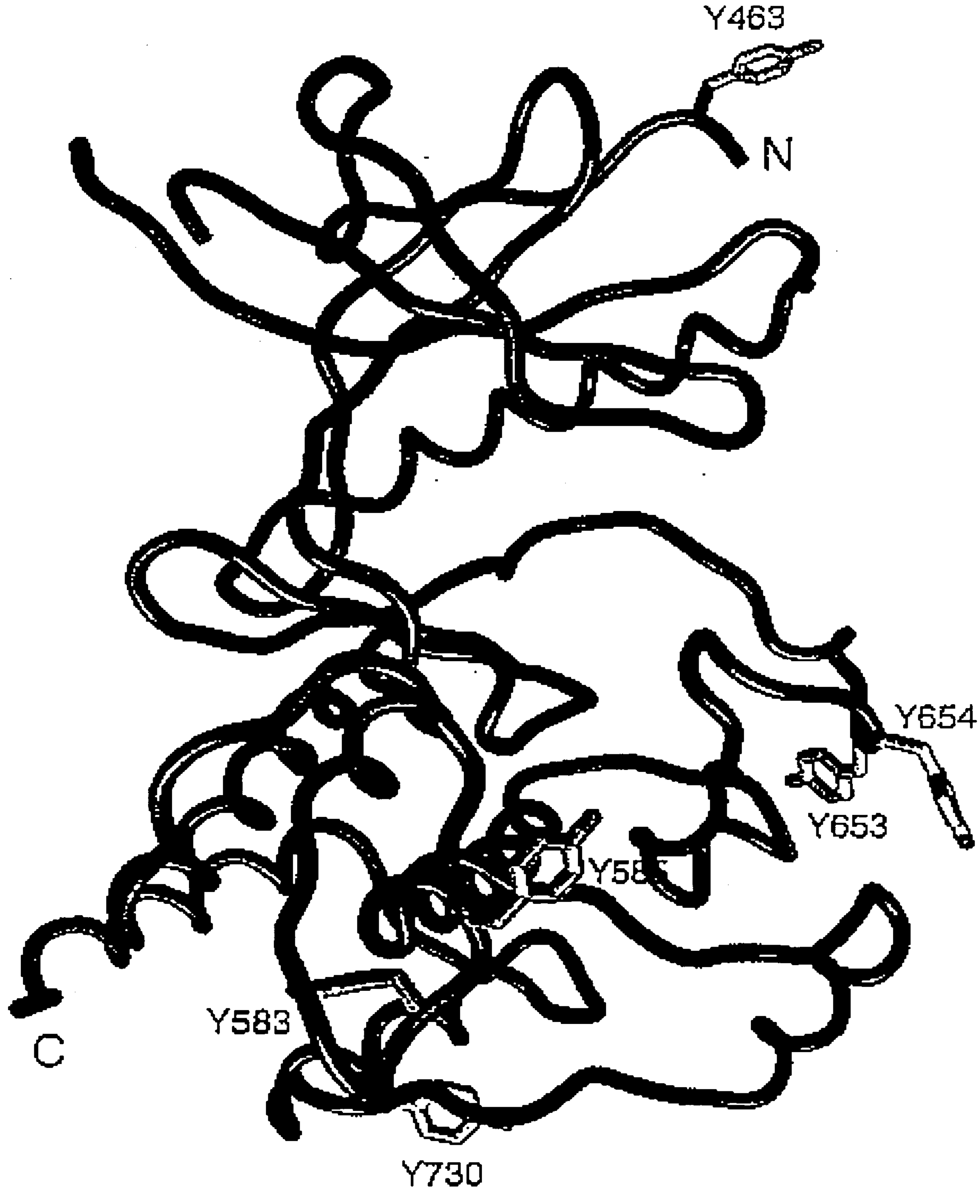


FIGURE 5

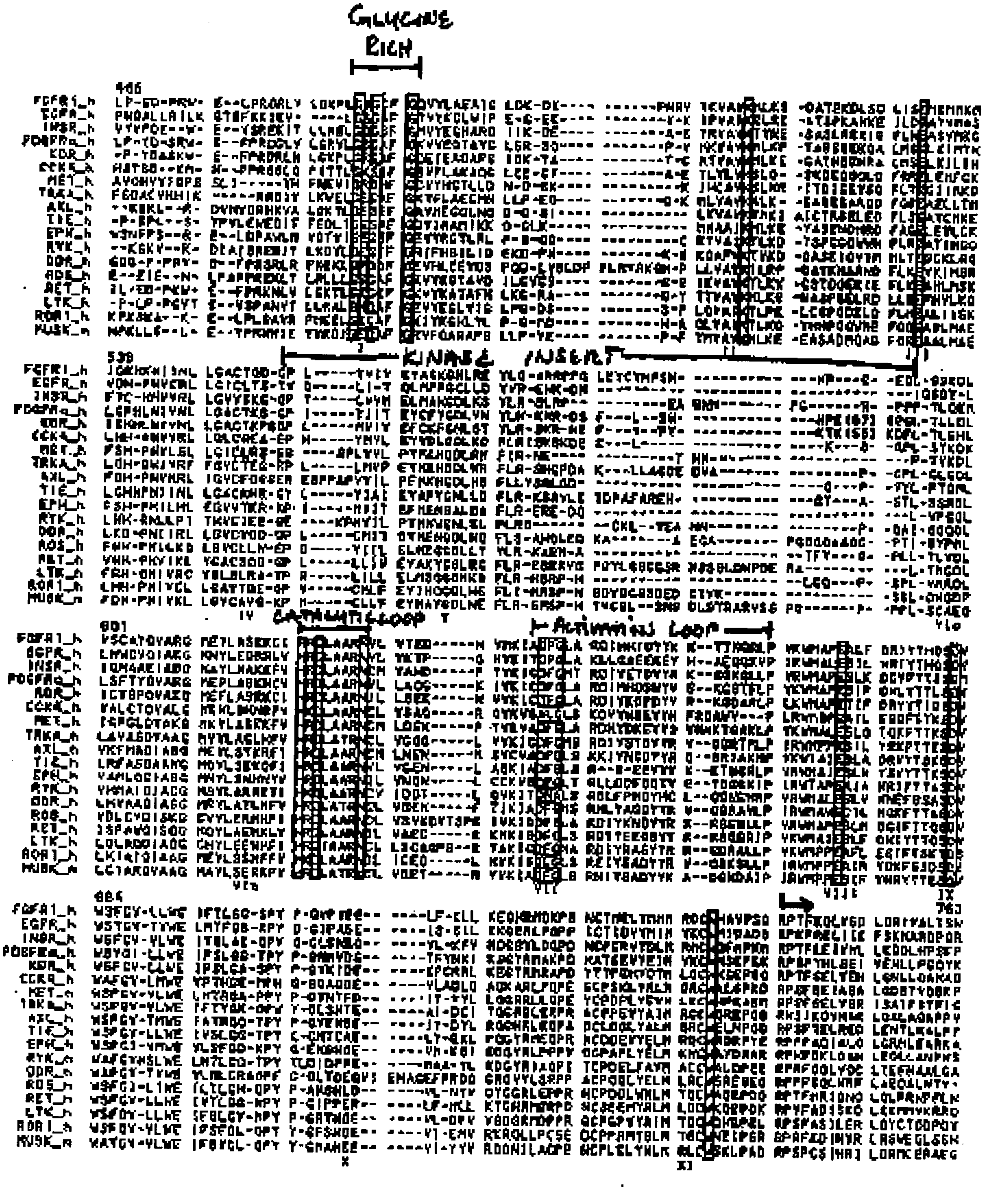

Glycine Rich
Kinase Insert
Catalytic Loop
Activation Loop
466
539
601
684
763
FGFR1_h
EGFR_h
INSR_h
PDGFRa_h
KDR_h
CCK4_h
MET_h
TRKA_h
AXL_h
TIE_h
EPH_h
RYK_h
DDR_h
ROS_h
RET_h
LTK_h
ROR1_h
MUSK_h

FIGURE 6A

```
         485
FGFR1_h  LPEDPRWELP RDRLVLGK-P LGEGCFGQVV LAEAIGLDKD KPNRVTKVAV KMLKSDATEK DLSDLISEME MMKMI-GKHK
  SRC_h  GLAKDAWEIP RESLRLEV-K LGQGCFGEVW MGTW------ NGT--TRVAI KTLKPGTMSP -E--AFLQ-E AQVMKKLRHE
  BRK_h  LPHVDDWERP REEFTLCR-K LGSGYFGEVF EGLW------ KDR--VQVAI KVISRDNLLH -Q--QMLQSE IQAMKKLRHK
  BTK_h  GLGYGSWEID PKDLTFLK-E LGTGQFGVVK YGKW------ RGQYD--VAI KMIKEGSMSE -D--EFIE-E AKVMMNLSHE
  CSK_h  EFYRSGWALN MKELKLLQ-T IGKGEFGDVM LGDY------ RGN---KVAV KCIKNDA-TA -Q--AFL-AE ASVMTQLRHS
  ABL_h  SPNYDKWEME RTDITMKH-K LGGGQYGEVY EGVW------ K-KYSLTVAV KTLKEDTMEV -E--EFLK-E AAVMKEIKHP
ZAP70_h  LKDKKLF-LK RDNLLIADIE LGCGNFGSVR QGVY----RM RKKQ-IDVAI KVLKQG--TE KADTEEMMRE AQIMHQLDNP
  FES_h  AVPKDKWVLN HEDLVLGE-Q IGRGNFGEVF SGR------- LRADNTLVAV KSCRETLPPD LKAK-FLQ-E ARILKQYSHP
  FAK_h  MPSTRDYEIQ RERIELGRC- IGEGQFGDVH QGIY----MS PENPALAVAI KTCKNC--TS DSVREKFLQE ALTMRQFDHP
 JAK1_h  PTEVDPTHFE KRFLKRIR-D LGEGHFGKVE LCRY----DP EGDNTGEQVA VKSLKPE--SG GNHIADLKKE IEILRNLYHE
  ACK_h  PLQSLTCLIG EKDLRLLE-K LGDGSFGVVR RGEW----DA PSGKTVSVAV KCLKPDVLSQ PEAMDDFIRE VNAMHSLDHR
                               I                            II                       III

         543
FGFR1_h  NIINLLGACT -QDGP-LYVI VEYASKGNLR EYLQARRPPG LEYCYNPSHN PEEQLSSKDL VSCAYQVARG MEYLASKKCI
  SRC_h  KLVQLYAVVS -E-EP-IYIV TEYMSKGSLL DFLKGET--- ---------- -GKYLRLPQL VDMAAQIASG MAYVERMNYV
  BRK_h  HILALYAVVS VG-DP-VYII TELMAKGSLL ELLRDSD--- ---------- -EKYLPVSEL LDIAWQVAEG MCYLESQNYI
  BTK_h  KLVQLYGVCT KQR-P-IFII TEYMANGCLL NYLRE-M--- ---------- -RHRFQTQQL LEMCKDVCEA MEYLESKQFL
  CSK_h  NLVQLLGVIV EEKGG-LYIV TEYMAKGSLV DYLRSRG--- ---------- -RSVLGGDCL LKFSLDVCEA MEYLEGNNFV
  ABL_h  NLVQLLGVCT REP-P-FYII TEFMTYGNLL DYLRECN--- ---------- -RQEVNAVVL LYMATQISSA MEYLEKKNFI
ZAP70_h  YIVRLIGVCQ AEA---LMLV MEMAGGGPLH KFLVGK---- ---------- -REEIPVSNV AELLHQVSMG MKYLEEKNFV
  FES_h  NIVRLIGVCT -QKQP-IYIV MELVQGGDFL TFLRTE---- ---------- -GARLRVKTL LQMVGDAAAG MEYLESKCCI
  FAK_h  HIVKLIGVIT ENP---VWII MELCTLGELR SFLQVR---- ---------- -KYSLDLASL ILYAYQLSTA LAYLESKRFV
 JAK1_h  NIVKYKGICT EDGGNGIKLI MEFLPSGSLK EYLPKN---- ---------- -KNKINLKQQ LKYAVQICKG MDYLGSRQYV
  ACK_h  NLIRLYGVVL TPP---MKMV TELAPLGSLL DRLRKH---- ---------- -QGHFLLGTL SRYAVQVAEG MGYLESKRFI
                   IV                V                                 VIa                   VIb

         621
FGFR1_h  HRDLAARNVL VTEDNVMKIA DFGLARDIH- HIDYYKKTTN GRLPVKWMAP EAL-FDRIYT HQSDVWSFGV LLWEIFTLGG
  SRC_h  HRDLRAANIL VGENLVCKVA DFGLARLIE- DNEYTARQGA -KFPIKWTAP EAALYGR-FT IKSDVWSFGI LLTELTTKGR
  BRK_h  HRDLAARNIL VGENTLCKVG DFGLARLIK- EDVYLSHD-H -NIPYKWTAP EALSRGH-YS TKSDVWSFGI LLHEMFSRGQ
  BTK_h  HRDLAARNCL VNDQGVVKVS DFGLSRYVL- DDEYTSSVGS -KFPVRWSPP EVLMYSK-FS SKSDIWAFGV LMWEIYSLGK
  CSK_h  HRDLAARNVL VSEDNVAKVS DFGLTK---- -EASSTQDTG -KLPVKWTAP EALREKK-FS TKSDVWSFGI LLWEIYSFGR
  ABL_h  HRDLAARNCL VGENHLVKVA DFGLSRLMT- GDTYTAHAGA -KFPIKWTAP ESLAYNK-FS IKSDVWAFGV LLWEIATYGM
ZAP70_h  HRDLAARNVL LVNRHYAKIS DFGLSKALGA DDSYYTARSA GKWPLKWYAP ECINFRK-FS SRSDVWSYGV TMWEALSYGQ
  FES_h  HRDLAARNCL VTEKNVLKIS DFGMSREEA- DGVYAASGGL RQVPVKWTAP EALNYGR-YS SESDVWSFGI LLWETFSLGA
  FAK_h  HRDIAARNVL VSSNDCVKLG DFGLSRYME- DSTYYKA-SK GKLPIKWMAP ESINFRR-FT SASDVWMFGV CMWEILMHGV
 JAK1_h  HRDLAARNVL VESEHQVKIG DFGLTKAIET DKEYYTVKDD RDSPVFWYAP ECLMQSK-FY IASDVWSFGV TLHELLTYCD
  ACK_h  HRDLAARNLL LATRDLVKIG DFGLMRALPQ NDDHYVMQEH RKVPFAWCAP ESLKTRT-FS HASDTWMFGV TLWEMFTYGQ
                                VII                             VIII           IX

         699                                                                              784
FGFR1_h  S--------- ----PYPGVP VEELFKLLKE -GHRMDKPSN CTNELYMMMR DCWHAVPSQR PTFKQLVEDL DRIVALTSNQ
  SRC_h  V--------- ----PYPGMV NREVLDQVER -GYRMPCPPE CPESLHDLMC QCWRKEPEER PTFEYLQAFL EDYFTSTEPQ
  BRK_h  V--------- ----PYPGMS NHEAFLRVDA -GYRMPCPLE CPPSVHKLML TCWCRDPEQR PCFKALRERL SSFTSYENPT
  BTK_h  M--------- ----PYERFT NSETAEHIAQ -GLRLYRPHL ASEKVYTIMY SCWHEKADER PTFKILLSNI LDVMDEES--
  CSK_h  V--------- ----PYPRIP LKDVVPRVEK -GYKMDAPDG CPPAVYEVMK NCWHLDAAMR PSFLQLREQL EHIKTHELHL
  ABL_h  S--------- ----PYPGID LSQVYELLEK -DYRMERPEG CPEKVYELMR ACWQWNPSDR PSFAEIHQAF ETMFQESSIS
ZAP70_h  K--------- ----PYKKMK GPEVMAFIE- QGKRMECPPE CPPELYALMS DCWIYKWEDR PDFLTVEQRM RACYYSLASK
  FES_h  S--------- ----PYPNLS NQQTREFVEK -GGRLPCPEL CPDAVFRLME QCWAYEPGQR PSFSTIYQEL QSIR--KRHR
  FAK_h  K--------- ----PFQGVK NNDVIGRIE- NGERLPMPPN CPPTLYSLMT KCWAYDPSRR PRFTELKAQL STILEEEKAQ
 JAK1_h  SDSSPMALFL KMIGPTHGQM TVTRLVNTLK EGKRLPCPPN CPDEVYQLMR KCWEFQPSNR TSFQNLIEGF -----EALLK
  ACK_h  E--------- ----PWIGLN GSQILHKIDK EGERLPRPED CPQDIYNVMV QCWAHKPEDR PTFVALRDFL LEAQPTDMRA
                            X                           XI
```

FIGURE 6B

CORRECTED VERSION*

PCT

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# INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(51) International Patent Classification $^6$ :
C12N 15/54, C07K 14/71, 14/705, C12N 9/12, 15/12, C12Q 1/48, G01N 33/68, C07D 209/34, A61K 31/40

A3

(11) International Publication Number: WO 98/07835

(43) International Publication Date: 26 February 1998 (26.02.98)

(21) International Application Number: PCT/US97/14885

(22) International Filing Date: 21 August 1997 (21.08.97)

(30) Priority Data:

| | | |
|---|---|---|
| 08/701,191 | 21 August 1996 (21.08.96) | US |
| 60/034,168 | 19 December 1996 (19.12.96) | US |

(60) Parent Application or Grant
(63) Related by Continuation
US Not furnished (CIP)
Filed on Not furnished

(71) Applicant *(for all designated States except US)*: SUGEN, INC. [US/US]; 351 Galveston Drive, Redwood City, CA 94063 (US).

(72) Inventors; and
(75) Inventors/Applicants *(for US only)*: MOHAMMADI, Moosa [IR/US]; 564 First Avenue #12F, New York, NY 10016 (US). LI, Sun [CN/US]; 64 Rockharbor Lane, Foster City, CA 94404 (US). LIANG, Congxin [CN/US]; 726 W. Remington Drive, Sunnyvale, CA 94087-2242 (US). SCHLESSINGER, Joseph [IL/US]; 37 Washington Square West, New York, NY 10011 (US). HUBBARD, Stevan, R. [US/US]; 5465 Sylvan Avenue, Riverdale, NY 10471 (US). McMAHON, Gerald [US/US]; 1800 Schultz Road, Kenwood, CA 95452 (US). TANG, Peng, C. [US/US]; 827 Camino Ricardo, Moraga, CA 94556 (US).

(74) Agents: WARBURG, Richard, J. et al.; Lyon & Lyon LLP, First Interstate World Center, Suite 4700, 633 West Fifth Street, Los Angeles, CA 90071-2066 (US).

(81) Designated States: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, ARIPO patent (GH, KE, LS, MW, SD, SZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG).

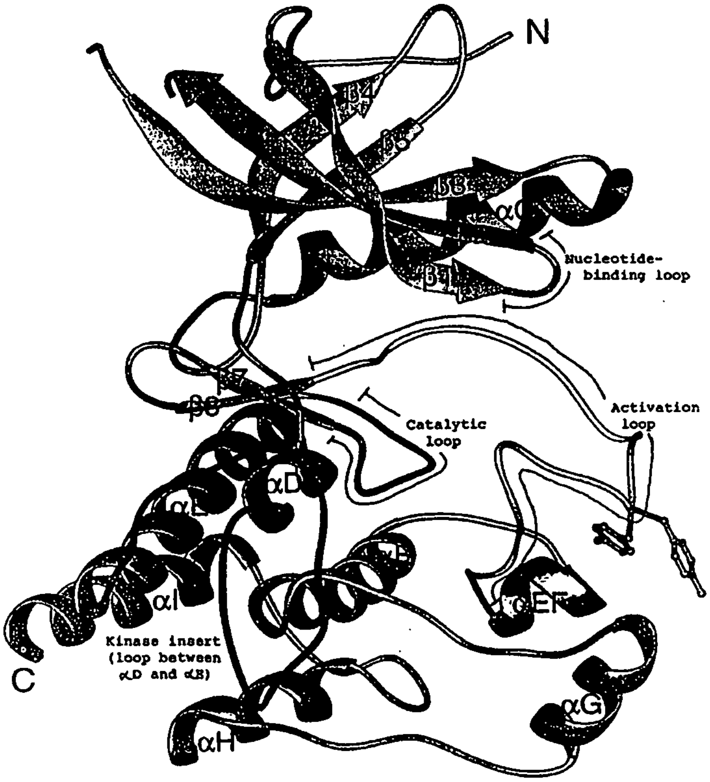
**Published**
*With international search report.*

(88) Date of publication of the international search report: 1 October 1998 (01.10.98)

## (54) Title: CRYSTAL STRUCTURES OF A PROTEIN TYROSINE KINASE

## (57) Abstract

The present invention relates to the three-dimensional structures of a protein tyrosine kinase optionally complexed with one or more compounds. The atomic coordinates that define the structures of the protein tyrosine kinase and any of the compounds bound to it are pertinent to methods for determining the three-dimensional structures of protein tyrosine kinases with unknown structure and to methods that identify modulators of protein tyrosine kinase functions.



*(Referred to in PCT Gazette No. 23/1998, Section II)

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| UZ | Uzbekistan |
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| ZW | Zimbabwe |

# INTERNATI[illegible]L SEARCH REPORT

Inte[illegible]l Application No
PCT/US 97/14885

**A. CLASSIFICATION OF SUBJECT MATTER**

IPC 6 C12N15/54 C07K14/71 C07K14/705 C12N9/12 C12N15/12
C12Q1/48 G01N33/68 C07D209/34 A61K31/40

According to International Patent Classification (IPC) or to both national classification and IPC

**B. FIELDS SEARCHED**

Minimum documentation searched (classification system followed by classification symbols)

IPC 6 C07K C12N

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

**C. DOCUMENTS CONSIDERED TO BE RELEVANT**

| Category ° | Citation of document, with indication, where appropriate, of the relevant passages | Relevant to claim No. |
|---|---|---|
| X | S. R. HUBBARD ET AL: "Crystal structure of the Tyrosine kinase domain of the human insulin receptor"<br>NATURE.,<br>vol. 372, 22 December 1994, LONDON GB,<br>pages 746-754, XP002061072<br>cited in the application<br>see the whole document<br>--- | 1,2,6,<br>24,25,30 |
| X | LEI WEI ET AL: "Expression, characterization , and crystallization of the catalytic core of the human insulin receptor protein-tyrosine kinase domain"<br>JOURNAL OF BIOLOGICAL CHEMISTRY.,<br>vol. 270, no. 14, 1995, MD US,<br>pages 8122-8130, XP002061073<br>see page 8129, last paragraph - page 8130<br>---<br>-/-- | 1,2,24,<br>25,30 |

☒ Further documents are listed in the continuation of box C.

☒ Patent family members are listed in annex.

° Special categories of cited documents :

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"P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

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"&" document member of the same patent family

| | |
|---|---|
| Date of the actual completion of the international search<br>17 April 1998 | Date of mailing of the international search report<br>27.07.1998 |
| Name and mailing address of the ISA<br>European Patent Office, P.B. 5818 Patentlaan 2<br>NL - 2280 HV Rijswijk<br>Tel. (+31-70) 340-2040, Tx. 31 651 epo nl,<br>Fax: (+31-70) 340-3016 | Authorized officer<br>LE CORNEC N.D.R. |

2

# INTERNA[illegible]ONAL SEARCH REPORT

[illegible]al Application No
PCT/US 97/14885

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

| Category ° | Citation of document, with indication,where appropriate, of the relevant passages | Relevant to claim No. |
|---|---|---|
| A | WO 92 13870 A (THE REGENTS OF THE UNIVERSITY OF CALIFORNIA) 20 August 1992<br>see claims 26-28<br>----- | 24,25,27 |

8

2

International application No.
PCT/US 97/14885

## INTERNATIONAL SEARCH REPORT

**Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)**

This International Search Report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claims Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:

2. ☐ Claims Nos.:
because they relate to parts of the International Application that do not comply with the prescribed requirements to such an extent that no meaningful International Search can be carried out, specifically:

3. ☐ Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

**Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)**

This International Searching Authority found multiple inventions in this international application, as follows:

see annex

1. ☐ As all required additional search fees were timely paid by the applicant, this International Search Report covers all searchable claims.

2. ☐ As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.

3. ☐ As only some of the required additional search fees were timely paid by the applicant, this International Search Report covers only those claims for which fees were paid, specifically claims Nos.:

4. ☒ No required additional search fees were timely paid by the applicant. Consequently, this International Search Report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

subject 1 (Please see Extra sheet)

**Remark on Protest**

☐ The additional search fees were accompanied by the applicant's protest.

☐ No protest accompanied the payment of additional search fees.

Form PCT/ISA/210 (continuation of first sheet (1)) (July 1992)

**FURTHER INFORMATION CONTINUED FROM PCT/ISA/**

1. Claims: 1-3, 6, 24-25, 27, 30 all partially

   Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: PDGF-R. The polypeptide and the method used to form the crystal.

2. Claims: 1-3, 6, 24-25, 27, 30 all partially .

   Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase:FLK/KDR. The polypeptide and the method used to form the crystal.

3. Claims: 1-3, 6, 24-25, 27, 30 all partially

   Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: CCK4. The polypeptide and the method used to form the crystal.

4. Claims: 1-3, 6, 24-25, 27, 30 all partially

   Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: MET. The polypeptide and the method used to form the crystal.

5. Claims: 1-3, 6, 24-25, 27, 30 all partially

   Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: TRKA. The polypeptide and the method used to form the crystal.

6. Claims: 1-3, 6, 24-25, 27, 30 all partially

   Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: AXL. The polypeptide and the method used to form the crystal.

7. Claims: 1-3, 6, 24-25, 27, 30 all partially

   Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: TIE. The polypeptide and the method used to form the crystal.

**FURTHER INFORMATION CONTINUED FROM PCT/ISA/**

8. Claims: 1-3, 6, 24-25, 27, 30 all partially

Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: EPH. The polypeptide and the method used to form the crystal.

9. Claims: 1-3, 6, 24-25, 27, 30 all partially

Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: RYK. The polypeptide and the method used to form the crystal.

10. Claims: 1-3, 6, 24-25, 27, 30 all partially

Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: DDR. The polypeptide and the method used to form the crystal.

11. Claims: 1-3, 6, 24-25, 27, 30 all partially

Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: ROS. The polypeptide and the method used to form the crystal.

12. Claims: 1-3, 6, 24-25, 27, 30 all partially

Crystalline form of a polypeptide corresponding to the catalytic domain of a protein tyrosine kinase receptor: RET. The polypeptide and the method used to form the crystal.

13. Claims: 1-3, 6, 24-25, 27, 30 all partially

Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: LTK. The polypeptide and the method used to form the crystal.

14. Claims: 1-3, 6, 24-25, 27, 30 all partially

Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: ROR1. The polypeptide and the method used to form the crystal.

15. Claims: 1-3, 6, 24-25, 27, 30 all partially

Crystalline form of a polypeptide corresponding to the catalytic domain of a receptor protein tyrosine kinase: MUSK.The polypeptide and the method used to form the crystal.

**FURTHER INFORMATION CONTINUED FROM PCT/ISA/**

16. Claims: 1,4-6, 24, 26, 28, 30 all partially.

    Crystalline form of a polypeptide corresponding to the catalytic domain of a non-receptor protein tyrosine kinase: SRC. The polypeptide and the method used to form the crystal.

17. Claims: 1,4-6, 24, 26, 28, 30 all partially.

    Crystalline form of a polypeptide corresponding to the catalytic domain of a non-receptor protein tyrosine kinase: BRK. The polypeptide and the method used to form the crystal.

18. Claims: 1,4-6, 24, 26, 28, 30 all partially.

    Crystalline form of a polypeptide corresponding to the catalytic domain of a non-receptor protein tyrosine kinase: BTK. The polypeptide and the method used to form the crystal.

19. Claims: 1,4-6, 24, 26, 28, 30 all partially.

    Crystalline form of a polypeptide corresponding to the catalytic domain of a non-receptor protein tyrosine kinase: CSK. The polypeptide and the method used to form the crystal.

20. Claims: 1,4-6, 24, 26, 28, 30 all partially.

    Crystalline form of a polypeptide corresponding to the catalytic domain of a non-receptor protein tyrosine kinase: ABL. The polypeptide and the method used to form the crystal.

21. Claims: 1,4-6, 24, 26, 28, 30 all partially.

    Crystalline form of a polypeptide corresponding to the catalytic domain of a non-receptor protein tyrosine kinase: ZAP70. The polypeptide and the method used to form the crystal.

22. Claims: 1,4-6, 24, 26, 28, 30 all partially.

    Crystalline form of a polypeptide corresponding to the catalytic domain of a non-receptor protein tyrosine kinase: FES. The polypeptide and the method used to form the crystal.

**FURTHER INFORMATION CONTINUED FROM PCT/ISA/**

23. Claims: 1,4-6, 24, 26, 28, 30 all partially.

Crystalline form of a polypeptide corresponding to the catalytic domain of a non-receptor protein tyrosine kinase: FAK. The polypeptide and the method used to form the crystal.

24. Claims: 1,4-6, 24, 26, 28, 30 all partially.

Crystalline form of a polypeptide corresponding to the catalytic domain of a non-receptor protein tyrosine kinase: JAK. The polypeptide and the method used to form the crystal.

25. Claims: 1,4-6, 24, 26, 28, 30 all partially.

Crystalline form of a polypeptide corresponding to the catalytic domain of a non-receptor protein tyrosine kinase: ACK. The polypeptide and the method used to form the crystal.

26. Claims: 1, 24-25, 27, 30 all partially and 7-23, 29, 31-34 all completely.

Crystalline form of a polypeptide corresponding to the catalytic domain of a FGF receptor protein tyrosine kinase which is complexed or not with a compound. The polypeptide (cDNA encoding it) and the method used to form the crystal. The cDNA encoding FGFR tyrosine kinase as in seq ID. no 5.

27. Claims: 35-42 completely

Method to determine the three dimensional structure of receptor and/or non-receptor tyrosine kinases.

28. Claims: 43-50

Method of identifying a potential modulator of protein tyrosine kinase function by using a three dimensional computer representation.

29. Claims: 51-54, 57 all completely and 58-61 all partially

A modulator of protein tyrosine kinase function and its use in a method of treating a disease.

**FURTHER INFORMATION CONTINUED FROM PCT/ISA/**

30. Claims: 55 completely and 58-61 all partially

Method of identifying a potential modulator of protein tyrosine kinase by comparing the level of protein kinase phosphorylation between cells not administered the potential modulator and cells administered said potential modulator.

31. Claims: 56 completely and 58-61 all partially

Method of identifying a potential modulator of protein tyrosine kinase by comparing the rate of cell growth between cells not administered the modulator and cells administered the modulator.

# INTERNAT[illegible]AL SEARCH REPORT

Inform[illegible]n on patent family members

Inte[illegible]al Application No
PCT/US 97/14885

| Patent document cited in search report | Publication date | Patent family member(s) | Publication date |
|---|---|---|---|
| WO 9213870 A | 20-08-1992 | AU 669328 B | 06-06-1996 |
| | | AU 1346792 A | 07-09-1992 |
| | | CA 2101632 A | 01-08-1992 |
| | | EP 0572505 A | 08-12-1993 |
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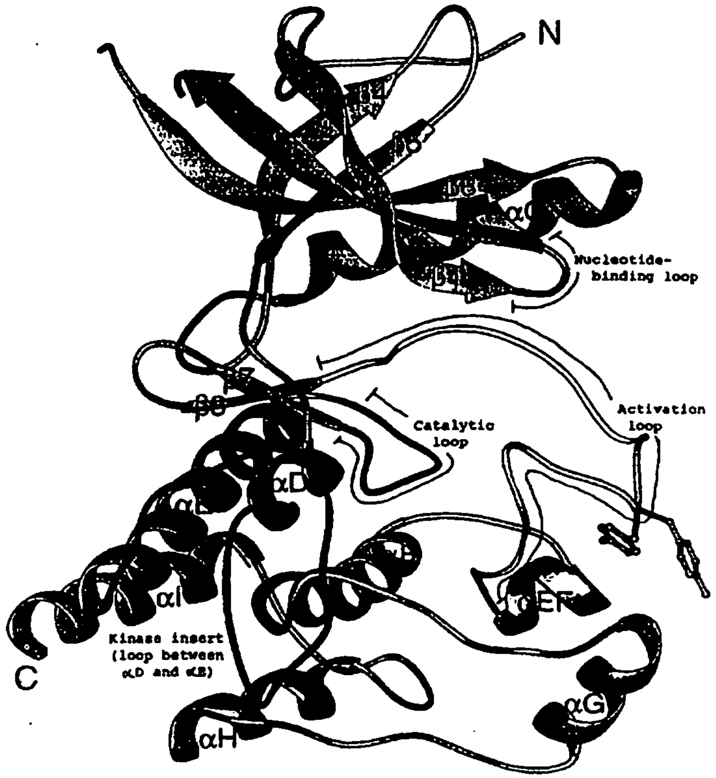
| | | JP 6505629 T | 30-06-1994 |
| | | NZ 241479 A | 27-09-1994 |


N
β4
β5
β3
αC
Nucleotide-binding loop
β1
β7
β8
Catalytic loop
Activation loop
αD
αE
αF
αEF
αI
Kinase insert (loop between αD and αE)
C
αG
αH